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(54) Title: SMALL MOLECULE MIMETICS OF ERYTHROPOIETIN  (57) Abstract  The invention features computer-assisted methods (100, 102, 104, 106, 200, 202, 204) for identifying molecules which will bind to the EPO receptor and act as an erythropoietin (EPO) mimetic. Preferred EPO mimetics identified using the method of the invention act as agonists of the EPO receptor in one or more <i>in vitro</i> or <i>in vivo</i> biological assays of EPO activity.			
<pre> graph TD     100[Input 3D coordinates of subset of EPO peptide] --&gt; 102[Compare subset to chemical database]     102 --&gt; 104[Select structurally similar chemical structures from database]     104 --&gt; 106[Output selected chemical structures]       </pre>			

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## SMALL MOLECULE MIMETICS OF ERYTHROPOIETIN

### BACKGROUND OF THE INVENTION

#### 1. *Field of the Invention*

This invention relates to computer-assisted methods for identifying and designing small molecule mimetics of erythropoietin.

#### 2. *Description of Related Art*

Erythropoietin (EPO) is the primary regulator of the proliferation and differentiation of immature erythroid cells. EPO is produced in the fetal liver and in the adult kidney in response to hypoxia (low oxygen levels in blood or tissue). It circulates in the blood stream where it targets the EPO receptor (EPOR) on committed progenitor cells in the bone marrow and other hematopoietic tissues. Recombinant human erythropoietin (rHuEPO) is widely used in therapy of patients with anaemia due to chronic renal failure, cancer chemotherapy and AZT treatment.

The EPO receptor belongs to the cytokine receptor superfamily which includes receptors for other hematopoietic growth factors such as interleukins (ILs), colony stimulating factors (CSFs) as well as growth hormone prolactin and ciliary neurotrophic factor (CNTF). The structural architecture of this family of receptors consists of three modules: a ligand binding extracellular domain, a short trans membrane region and a large cytoplasmic domain. It has been proposed that the extracellular domain of this superfamily comprises two discrete domains each containing approximately 100 residues that fold into a sandwich consisting of 7 antiparallel  $\beta$ -strands with the topology of an Ig constant domain. Members of the family share two characteristic motifs in their extracellular domain: a pair of conserved disulfide bridges in the N-terminal domain, and a WSXWS box (where X is any amino acid residue) in the C-terminal domain. For most members of this receptor superfamily, oligomerization of one or more polypeptide chains

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is essential for forming high affinity receptor complexes. A homodimer complex has been demonstrated to be the active form of hGHR and a similar model has been suggested for G-CSF, prolactin and EPO receptors.

5 Erythropoietin induces dimerization of two EPO receptor molecules, which results in subsequent phosphorylation of the cytoplasmic domains by the association with two tyrosine kinase (JAK2) molecules to initiate a cascade of events that leads to the relevant biological.

10 Given the importance of erythropoietin, it would be very desirable to be able to identify molecules capable of binding the EPO receptor and eliciting the response normally elicited by EPO.



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## SUMMARY OF THE INVENTION

The invention features methods for identifying molecules which will bind to the EPO receptor and act as a EPO mimetic. Preferred EPO mimetics identified using the method of the invention act as agonists of the EPO receptor in one or more *in vitro* or *in vivo* biological assays of EPO activity. Preferred mimetics are molecules lacking peptide bonds, i.e., are non peptidic mimetics. Preferred peptide mimetics have 15 or fewer, more preferably 10 or fewer amino acids.

The methods of the invention entail identification and design of molecules having a particular structure. The methods rely on the use of precise structural information derived from x-ray crystallographic studies of the extracellular domain of EPO receptor (amino acids 1 to 225) complexed with a peptide, EMP1 (EPO Mimetic Peptide 1; described below), which acts as an EPO mimetic. This crystallographic data permits the identification of atoms in the peptide mimetic that are important for EPO receptor binding and dimerization. More importantly, this data defines a three dimensional array of the important contact atoms. Other molecules which include a portion in which the atoms have a similar three dimensional arrangement similar to some or all of these contact atoms are likely to be capable of acting as an EPO mimetic. Moreover, one can use the structural information to design or identify molecules having even more EPO activity than the peptide mimetic described herein.

The details of the preferred embodiment of the present invention are set forth in the accompanying drawings and the description below. Once the details of the invention are known, numerous additional innovations and changes will become obvious to one skilled in the art.

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# **BRIEF DESCRIPTION OF THE DRAWINGS**

FIGURE 1 is a flowchart showing a first method for identifying potential mimetics of erythropoietin using a computer system.

5      FIGURE 2 is a flowchart showing a second method for identifying potential mimetics of erythropoietin using a computer system.

Like reference numbers and designations in the various drawings indicate like elements.

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## DETAILED DESCRIPTION OF THE INVENTION

Throughout this description, the preferred embodiment and examples shown should be considered as exemplars, rather than as limitations on the present invention.

Described below is the crystal structure of a small peptide mimetic of EPO bound to an  
5 extracellular portion of the EPO receptor. The peptide, EMP1  
(GGTYSCHFGPLTWVCKPQGG; SEQ ID NO:1), is characterized by an intramolecular  
disulfide bridge. Several lines of evidence suggest that EMP1 can act as an EPO mimetic.  
For example, EMP1 competes with EPO in receptor binding assays and induces cellular  
proliferation of cell lines engineered to be responsive to EPO. Both EPO and peptide  
10 induce a similar cascade of phosphorylation events and cell cycle progression in EPO  
responsive cells. Further, EMP1 demonstrates significant erythropoietic effects in mice  
as monitored by two different *in vivo* assays of nascent red blood cell production. This  
data, when combined, strongly supports the notion that the peptide ligand, which has a  
sequence unrelated to that of EPO, is capable of binding to and inducing an agonist  
15 conformation or assembly of EPO receptor.

### Design of small molecule mimetics

The structure of the EMP1 dimer demonstrates that a molecule substantially smaller than  
the natural hormone can act as an agonist and induce the appropriate biological response.  
The peptide is assumed to have a substantially smaller contact interface with the receptor  
20 than its natural hormone. The binding determinants in the EPO receptor form an almost  
flat surface which is mainly hydrophobic in nature, without any cavities or charged  
residues that may help in design of a small molecule ligand to interact with the receptor.

This simplified framework of interactions revealed by the structural data presented herein  
can be used to identify additional EPO mimetics. The atoms of EMP1 which are  
25 important for binding to the EPO receptor and forming dimeric EPO receptor include  
those involved in the contact between the EMP1 (peptide) and EBP (EPO receptor) and

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those involved in contacts between the two EMP1 molecules in the dimeric complex (peptide-peptide contacts). In addition to the contacts listed in Table 2, the following EMP1-EMP1 hydrophobic contacts are significant: Tyr<sup>P4</sup>, Cys<sup>P6</sup>, Phe<sup>P8</sup>, Trp<sup>P13</sup>, and Cys<sup>P15</sup> in each peptide. The following EMP1-EBP hydrophobic interactions are also significant: Tyr<sup>P4</sup>, Phe<sup>P8</sup>, and Trp<sup>P13</sup> in each peptide. It will be understood by those skilled in the art that not all of the atoms present in a significant contact residue need be present in a mimetic. In fact, it is only those few atoms which actually form important contacts with the EPO receptor which are likely to be important for mimetic activity. Those skilled in the art will be able to identify these important atoms based on the model of the dimeric EMP1-EPO complex which can be constructed using the structural data herein.

Preferred mimetics will include atoms at positions similar to those of the EPO receptor contacting atoms of EMP1. Even more preferred mimetics will be structurally similar to the dimer of EMP1 found in the structure described below. This is because the dimerization of EMP1 is an important factor in the dimerization of the EPO receptor.

The methods of the invention employ a computer-based methods for identifying compounds having a desired structure. More specifically, the invention uses the three-dimensional coordinates of a subset of the atoms in the peptide GGTYSCHFGLTWVCKPQGG when the peptide is co-crystallized with a portion of the erythropoietin receptor comprising amino acids 1 to 225 of the human EPO receptor, to determine peptide and non-peptide mimetic candidates by means of computer methods.

These computer-based methods fall into two broad classes: database methods and *de novo* design methods. In database methods the compound of interest is compared to all compounds present in a database of chemical structures and compounds whose structure is in some way similar to the compound of interest are identified. The structures in the database are based on either experimental data, generated by NMR or x-ray crystallography, or modeled three-dimensional structures based on two-dimensional (*i.e.*, sequence)

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data. In *de novo* design methods, models of compounds whose structure is in some way similar to the compound of interest are generated by a computer program using information derived from known structures, *e.g.*, data generated by x-ray crystallography and/or theoretical rules. Such design methods can build a compound having a desired structure in either an atom-by-atom manner or by assembling stored small molecular fragments.

The success of both database and *de novo* methods in identifying compounds with activities similar to the compound of interest depends on the identification of the functionally relevant portion of the compound of interest. For drugs, the functionally relevant portion is referred to a pharmacophore. A pharmacophore then is an arrangement of structural features and functional groups important for biological activity, *e.g.*, EPO activity.

Not all identified compounds having the desired pharmacophore will act as an EPO mimetic. The actual activity can be finally determined only by measuring the activity of the compound in relevant biological assays. However, the methods of the invention are extremely valuable because they can be used to greatly reduce the number of compounds which must be tested to identify an actual mimetic.

Dimerization of the EPO receptor is important for activity. Accordingly, preferred mimetics will be based on the structure of the EMP1 dimer as it is bound to the EPO receptor dimer. Thus, preferred mimetics have include important contacts from both of the RWJ 61233 peptides present in the structure described below. Such mimetics will favor dimerization of the EPO receptor.

Programs suitable for generating predicted three-dimensional structures from two-dimensional data include: Concord (Tripos Associated, St. Louis, MO), 3-D Builder (Chemical Design Ltd., Oxford, U.K.), Catalyst (Bio-CAD Corp., Mountain View, CA), and Daylight (Abbott Laboratories, Abbott Park, IL).

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Programs suitable for searching three-dimensional databases to identify molecules bearing a desired pharmacophore include: MACCS-3D and ISIS/3D (Molecular Design Ltd., San Leandro, CA), ChemDBS-3D (Chemical Design Ltd., Oxford, U.K.), and Sybyl/3DB Unity (Tripos Associates, St. Louis, MO).

- 5 Programs suitable for pharmacophore selection and design include: DISCO (Abbott Laboratories, Abbott Park, IL), Catalyst (Bio-CAD Corp., Mountain View, CA), and ChemDBS-3D (Chemical Design Ltd., Oxford, U.K.).

Databases of chemical structures are available from Cambridge Crystallographic Data Centre (Cambridge, U.K.) and Chemical Abstracts Service (Columbus, OH).

- 10 *De novo* design programs include Ludi (Biosym Technologies Inc., San Diego, CA) and Aladdin (Daylight Chemical Information Systems, Irvine CA).

Those skilled in the art will recognize that the design of a mimetic may require slight structural alteration or adjustment of a chemical structure designed or identified using the methods of the invention.

- 15 In general, chemical compounds identified or designed using the methods of the invention can be synthesized chemically and then tested for EPO activity using any of the methods described below. The methods of the invention are particularly useful because they can be used to greatly decrease the number potential mimetics which must be screened for EPO activity.

- 20 The invention may be implemented in hardware or software, or a combination of both. However, preferably, the invention is implemented in computer programs executing on programmable computers each comprising a processor, a data storage system (including volatile and non-volatile memory and/or storage elements), at least one input device, and at least one output device. Program code is applied to input data to perform the functions

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described above and generate output information. The output information is applied to one or more output devices, in known fashion. The computer may be, for example, a personal computer, microcomputer, or workstation of conventional design.

Each program is preferably implemented in a high level procedural or object oriented programming language to communicate with a computer system. However, the programs can be implemented in assembly or machine language, if desired. In any case, the language may be a compiled or interpreted language.

Each such computer program is preferably stored on a storage media or device (e.g., ROM or magnetic diskette) readable by a general or special purpose programmable computer, for configuring and operating the computer when the storage media or device is read by the computer to perform the procedures described herein. The inventive system may also be considered to be implemented as a computer-readable storage medium, configured with a computer program, where the storage medium so configured causes a computer to operate in a specific and predefined manner to perform the functions described herein.

FIGURE 1 is a flowchart showing a first method for identifying potential mimetics of erythropoietin using a computer system. The method uses a programmed computer comprising a processor, a data storage system, at least one input device, and at least one output device, and comprises the steps of:

- (1) inputting into the programmed computer through an input device data comprising the three-dimensional coordinates of a subset of the atoms in the peptide GGTYSCHFGPLTWVCKPQGG when the peptide is co-crystallized with a portion of the erythropoietin receptor comprising amino acids 1 to 225 of the receptor, thereby generating a criteria data set (STEP 100);
- (2) comparing, using the processor, the criteria data set to a computer database of chemical structures stored in the computer data storage system (STEP 102);

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- (3) selecting from the database, using a program suitable for searching three-dimensional databases to identify molecules bearing a desired pharmacophore (such as those described above or equivalents), chemical structures having a portion that is structurally similar to the criteria data set (STEP 104);
- 5 (4) outputting to an output device the selected chemical structures having a portion similar to the criteria data set (STEP 106).

FIGURE 2 is a flowchart showing a second method for identifying potential mimetics of erythropoietin using a computer system. The method uses a programmed computer comprising a processor, a data storage system, at least one input device, and at least one  
10 output device, and comprises the steps of:

- (1) inputting into the programmed computer through an input device data comprising the three-dimensional coordinates of a subset of the atoms in the peptide GGTYSCHFGPLTWVCKPQGG when the peptide is co-crystallized with a portion of the erythropoietin receptor comprising amino acids 1 to 225 of the  
15 receptor, thereby generating a criteria data set (STEP 200);
- (2) constructing, using a program suitable for generating chemical structure models (such as those described above or equivalents), a model of a chemical structure having a portion that is structurally similar to the criteria data set (STEP 202);
- (3) outputting to the output device the constructed model (STEP 204).

## 20 Confirmation of Biological Activity

In order to determine whether a molecule identified using the methods of the invention can act as an EPO mimetic, one or more *in vitro* or *in vivo* assays of EPO activity should be performed. For example, mimetic molecules should be able to stimulate proliferation of TF-1 cells (Kitamura et al., J. Cell Physiol. 140:323, 1985) or  
25 B6Sut cells (Greenberger et al., Proc. Natl. Acad. Sci. USA 80:2931, 1983), but preferably do not stimulate proliferation of cells which do not bear the EPO receptor. Thus, preferred mimetics do not stimulate proliferation of Mo7e cells (Avanzi et al., Br. J. Haematol. 69:359, 1988).



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Potential mimetics can also be tested in a murine model of erythropoiesis. In this assay a potential mimetic is administered to normal mice which express endogenous basal levels of EPO. Reticulocytes are counted, preferably by flow cytometry, to determine whether the candidate mimetic increases reticulocyte levels. An increase in reticulocyte levels indicates that the candidate mimetic is stimulating erythropoiesis. Because the mice used in this assay already express EPO, this assay may be relatively insensitive. As an alternative, candidate mimetics can be assayed in the exhypoxic-polycythemic mouse bioassay. In this assay polycythemia is induced by conditioning mice in a hypobaric chamber to reduce endogenous EPO levels. A potential EPO mimetic can be administered to a conditioned mouse. Incorporation of  $^{59}\text{Fe}$  into blood serves as a measure of erythropoiesis. This erythropoiesis can be attributed to the candidate mimetic.

The assays described above are examples of suitable assays. Other assays for EPO activity known to those skilled in the art are also useful.

In order to determine the biological activity of a candidate mimetic it is preferable to measure biological activity at several concentrations of candidate mimetic. The activity at a given concentration of candidate mimetic can be compared to the activity of EPO itself.

#### Structural Data

The coordinates for amino acids 1 to 225 of the human EPO receptor bound to peptide EMP1 are presented in the attached appendix in standard Brookhaven database format. Also included in this appendix is a list of van der Waals interactions. These coordinates can be used in the design and identification of EPO mimetics according to the methods of the invention.

#### Structure of EBP-EMP1 Complex

The extracellular fragment of human EPO receptor (EPO binding protein, EBP), consisting of residues 1-225, was expressed in Escherichia coli and purified as described

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(Johnson et al., Protein Express. Purif. 7:104, 1996). Rhomboidal-shaped crystals of an EBP complex with EMP1 were obtained in orthorhombic space group P2<sub>1</sub>2<sub>1</sub>2<sub>1</sub>, with cell parameters a=59.2Å, b=75.5Å, c=132.2Å, with two EBP and two peptide molecules in the asymmetric unit and a V<sub>m</sub>=2.8 Å<sup>3</sup>/dalton (Matthews, J. Mol. Biol. 33:491, 1968). The  
5 crystal structure was determined by multiple isomorphous replacement (MIR) using two heavy atom derivatives (Table 1). Residues 1-2 and 19-20 of each peptide as well as residues 1-9, 21-23, 164-166, 221-225 of receptor molecule I, and residues 1-9, 21-23, 133-135, 221-225 of receptor molecule II had poor or no electron density and are excluded from the structure analyses

10 An important break in the electron density that affects the structure interpretation occurs for the three residues (Arg<sup>21</sup>-Gly<sup>22</sup>-Pro<sup>23</sup>) that link the amino terminal α-helix to the first β-strand in D1 of both receptor molecules. A molecular packing diagram shows the proximity of a second non-crystallographically related dimer in the crystal that gives two possibilities of how this three-residue linker may be connected. The current choice of  
15 linker connectivity is based on a structure of another independent EBP-peptide complex at higher resolution (2.5 Å), which shares a similar molecular packing, but for which the electron density is clear for these three residues. At present there are no experimental data to verify whether this N-terminal α-helix exists in solution or is a crystallization packing artifact. Notably, this helical region is not observed in the published structures  
20 of hGHbp (begins at residue 32; deVos et al., Science 255:306, 1992), PRLR (begins at residue 2, without any defined secondary structure until the first β-strand, residue 6; Somers et al., Nature 372:478, 1994), the INF-γRα (begins at residue 17; Walter et al., Nature 376:230, 1995) or the tissue factor (begins at residue 3 without any defined secondary structure until the first β-strand, residue 11; Muller et al., Nature 370:662,  
25 1994).

The EBP monomer folds into two domains, D1 and D2, that form an L-shape with the long axis of each domain aligned at approximately 90° to each other; the overall molecular dimensions are 45 Å x 52 Å x 62 Å. The N-terminal domain (D1, residues 10-

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114) and C-terminal domain (D2, residues 119-220) are connected by a short four residue  $\alpha$ -helix linker. Both domains are more closely related in overall topology to Fibronectin type-III (FBN-III) domains than to Ig domains (Bork et al., *J. Mol. Biol.*, 242:309, 1994). The FBN-III fold is composed of two antiparallel  $\beta$ -pleated sheets, consisting of strands A, B, E and strands G, F, C and C', and is found in the two domains of the human growth hormone (de Vos et al., *Science* 255:306, 1992) and prolactin (Somers et al., *Nature* 372:478, 1994) receptors, the D1 and D2 domains of the  $\alpha$  chain of interferon- $\gamma$  receptor (IFN- $\gamma$ R $\alpha$ ) (Walter et al., *Nature* 376:230, 1995), the D2 domain of CD4 (Wang et al., *Nature* 348:411, 1990; Ryu et al., *Nature* 348:419, 1990), the two domains of tissue factor (Muller et al., *Biochemistry* 33:10864, 1994; Harlos et al., *Nature* 370:662, 1994), the third fibronectin-type repeat of tenascin (Leagy et al., *Science* 258:987, 1992) and the D2 domain of the chaperone protein PapD (Holmgren et al., *Nature* 342:248, 1989). The FBN-III topology differs from an Ig constant domain by a shift of strand D from one  $\beta$ -sheet (strands A, B, E and D) to the other (strands G, F, C, C'), where it is defined as the C' strand. Superposition of equivalent  $\beta$ -sheet core residues of the D1 and D2 domains in EBP gives an r.m.s. deviation of 2.3 Å for 77 C $\alpha$  pairs, which is significantly larger than the corresponding domain overlaps for hGHbp (1.1Å) and PRLR (0.8Å), and reflects a difference in the subclass of fold between the two EBP domains.

In D1, a short  $\alpha$ -helix (residues 10-20), precedes the first  $\beta$ -sandwich that is better described as a hybrid of the FBN-III fold with an Ig fold (residues 24-114), rather than strict FBN-III topology. In this h-type fold (Wang et al., *Nature* 348:411, 1990; Ryu et al., *Nature* 348:419, 1990), the C' strand is long and interacts first with strand C and then switches to interact with strand E (where C' changes its designation to strand D) forming a four-on-four strand  $\beta$ -sandwich. D1 contains the two conserved disulfide bridges linking Cys<sup>24</sup> ( $\beta$ A) to Cys<sup>33</sup> ( $\beta$ B) and Cys<sup>67</sup> ( $\beta$ C') to Cys<sup>76</sup> ( $\beta$ E). The number of residues between the cysteine pairs that form the two disulfide bridges are 9 and 15 for EBP, compared to 9 and 10 in both GHR and PRLR. The longer connection between strands C' and E enables the second half of strand C' to become strand D. This h-type topology is not found in either of the two s-type GHR domains. A potential glycoylation site exists

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on residue Asn<sup>52</sup> which is located towards the end of the loop region connecting the  $\beta$ B and  $\beta$ C strands. Although Asn<sup>52</sup> is not glycosylated in this bacterially expressed protein, an external cavity around the Asn<sup>52</sup> side chain could easily accommodate a carbohydrate moiety.

5 A helical linker (residues 115-118) connects D1 to D2 (The  $\phi$ ,  $\Psi$  torsion angles for the interdomain helical linker for Ile<sup>115</sup>, Asn<sup>116</sup>, Glu<sup>117</sup> and Val<sup>118</sup> are  $-50^\circ$ ,  $-27^\circ$ ,  $-76^\circ$ ,  $-21^\circ$ ,  $-99^\circ$ ,  $26^\circ$ , and  $-151^\circ$ ,  $38^\circ$  respectively.) and has been observed in other members of this receptor family, hGHbp, PRLR, IFN- $\gamma$ R $\alpha$  and tissue factor. In EBP, the domain association is further restricted by a mixed assortment of hydrogen bonding, hydrophobic  
10 interactions and one salt bridge (between Arg<sup>121</sup> and Asp<sup>122</sup>) from 11 residues of D1 and 12 residues of D2 with a total buried surface [The molecular surface areas buried by interaction were calculated using the program MS (Connolly, J. Appl. Crystallog, 16:439, 1983) using a 1.7Å probe sphere and standard atomic radii (as described in Davies, et al, Ann. Rev. Biochem. 59:439, 1990). There may be some discrepancies between values  
15 reported here and other (deVos et al., Science 255:306, 1992) published values due to use of a different algorithm (Connolly) vs. Lee et al., J. Mol. Biol., 55: 379, 1971) and probe radii. For clarity all values reported here have been calculated in the same way for better comparison between the receptors] of 950 Å<sup>2</sup> for the two domains.

D2 (residues 119-220) folds into the standard FBN-III (s-type) topology with one free  
20 cysteine and no disulfide bridges, consistent with GHR and PRLR that have three and two disulfide bridges, respectively, in D1 but none in D2. After the  $\alpha$ -helix linker, D2 begins with an irregular coil (residues 118-126) that contains Pro<sup>124</sup> which is conserved in the structures of hGHbp, PRLR, tissue factor and IFN $\gamma$ -R $\alpha$ , and based on sequence alignment, in most class-1 and class-2 cytokine receptors (Bazan, Proc. Natl. Acad. Sci.  
25 USA 87:6934, 1990). This short coil ends with Gly<sup>124</sup> which has a positive  $\phi$  ( $\phi$ ,  $\Psi$  =  $52^\circ$ ,  $40^\circ$ ) consistent with the equivalent Ala<sup>136</sup> and Ala<sup>101</sup> torsion angles in hGHbp ( $\phi$ ,  $\Psi$  =  $63^\circ$ ,  $68^\circ$ ) and PRLR ( $\phi$ ,  $\Psi$  =  $58^\circ$ ,  $38^\circ$ ). The Pro<sup>124</sup> region forms an analogous extended bulge conformation adjacent and parallel to a corresponding bulge containing the

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WSXWS motif. The WSAWS sequence forms a modified wide  $\beta$ -bulge (Richardson, Adv. Prot. Chem. 34:167, 1981) and is located in an extended chain region immediately preceding the  $\beta$ G strand that would normally connect to the membrane spanning region of the EPOR.

- 5 The quaternary structure of the complex is composed of two peptides and two receptors that form a T-shapes assembly. A noncovalent peptide dimer interacts with two receptor molecules to generate an almost perfect 2-fold symmetrical arrangement. After superposition of D2 of the two EBP molecules in the dimer, the centers of mass of the two D1 domains are only 0.8 Å apart, sufficient to perturb perfect two-fold symmetry.
- 10 Separate superposition of the corresponding D1 and D2 of each receptor in the dimer results in r.m.s. deviations of 0.53 Å (105 D1 C $\alpha$  pairs) and 0.47 Å (93 D2 C $\alpha$  pairs).

The cyclic EMP1 contains a single disulfide bridge between Cys<sup>P6</sup> and Cys<sup>P13</sup>, which links two short  $\beta$ -strands (residues 4-7 and 13-16) that are connected by a slightly distorted type I  $\beta$ -turn [Pro<sup>P10</sup> (i+1) and Leu<sup>P11</sup> (i+2) of the  $\beta$ -turn have  $\phi, \Psi \approx -62^\circ, -38^\circ$  and  $-99^\circ, -60^\circ$ , respectively. The carbonyl oxygen of Leu<sup>P11</sup> has a hydrogen bond to EBP distorting the  $\Psi$  value from its normal  $0^\circ \pm 30^\circ$  (i+2) in a standard type I  $\beta$ -turn.] consisting of residues Gly<sup>P9</sup>-Pro<sup>P10</sup>-Leu<sup>P11</sup>-Thr<sup>P12</sup>. Each peptide has a very close association with its other peptide partner and buries 320 Å<sup>2</sup> of its 1220 Å<sup>2</sup> molecular surface in this interaction (Connelly, J. Appl. Crystallog. 16:439, 1983; Davies et al., Ann. Rev. Biochem. 59:439, 1990; Richards, J. Mol. Biol. 55:379, 1971). Four hydrogen bonds between the mainchains of the two peptides results in formation of a four-stranded anti-parallel  $\beta$ -pleated sheet (Table 2). Two symmetric hydrophobic cores are assembled by peptide dimerization and are comprised of the disulfide bridges and the side chains of Tyr<sup>P4</sup>, Phe<sup>P8</sup> and Trp<sup>P13</sup>. The construction of each hydrophobic core resembles a box which places the aromatic rings of Phe<sup>P8</sup>, Trp<sup>P13</sup> and Tyr<sup>P4</sup> (from the other peptide) and the disulfide bridge (Cys<sup>P6</sup>-Cys<sup>P13</sup>) at the corners. The two glycine residues at either end of the peptide are not structured.

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The peptide dimer is embedded in a deep crevice between two EBP receptor molecules. A portion of each peptide monomer interacts with both receptor molecules. The binding sites of each EBP are practically identical due to the 2-fold symmetric interactions imposed on binding the peptide dimer. The four major contact areas on EBP come from segments on four loop regions (L1, L3, L5, L6) that connect strands A to B (L1 residues 33-34) and F to G (L6 residues 90-94) in D1 and strands B to C (L5 residues 148-153) and F to G (L6 residues 203-205) in D2. The total buried molecular surfaces in the peptide-EBP assembly are 840 Å<sup>2</sup> and 880 Å<sup>2</sup> for the two peptides and EBP's, respectively. The peptide-EBP interaction can be separated into distinct hydrophobic (67%) and polar (33%) areas. A hydrophobic core is formed between the peptide and receptor and comprises Phe<sup>93</sup>, Met<sup>150</sup> and Phe<sup>203</sup> from one EBP molecule and the peptide hydrophobic box consisting of Phe<sup>P8</sup> and Trp<sup>P13</sup> from one peptide and Tyr<sup>P4</sup> and Cys<sup>P15</sup> from the other peptide. The polar interactions are located mainly at the bottom of the binding crevice and are mainly with loop L5 in D2. Five of the six hydrogen bonds are between the mainchain of the β-turn residues Gly<sup>P9</sup>, Pro<sup>P10</sup> and Leu<sup>P11</sup> from one peptide with the mainchain and sidechain hydroxyl of conserved Tyr<sup>P4</sup>, which crosses over its other peptide partner, to interact with loop L3 (Table 2). The EBP-EBP interaction makes a surprisingly minor contribution to the overall stability of the complex where the inter-receptor buried molecular surface is only 75 Å<sup>2</sup>, contributed by Leu<sup>175</sup> and Arg<sup>178</sup> from each receptor molecule.

EMP1 is one of a family of sequences that contain several conserved residues, besides the cysteines (~~Hansen, Ann. Rev. Microbiol. 47:595, 1999~~). The most structurally significant of these consensus residues appear to be Tyr<sup>P4</sup> and Trp<sup>P13</sup>, which along with the disulfide bridge have a major contribution to the hydrophobic core of the peptide-peptide interaction. Moreover, these two aromatic residues play a pivotal role in peptide-receptor interaction and in receptor dimerization.

#### Dimerization of EBP in Solution

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To explore the interaction of EMP1 with EBP in solution we employed a bifunctional sulphhydryl reactive crosslinker DPDPB, [1,4-di-(2'-pyridyldithio propionamido) butane], in an attempt to stabilize a peptide-dependent dimeric structure. The choice of crosslinker was based on previous experiments with amine-reactive crosslinkers that were found to inactivate EBP. EBP contains a single free sulphhydryl (Cys<sup>181</sup>) in D2 which is potentially reactive to crosslinking reagents (The DPDPB crosslinker itself does not inactivate the EPO binding potential of EBP nor the proliferative properties of EMP1). A dimeric EBP product is formed by co-incubation of EMP1, DPDPB and EBP. The amount of dimeric product increases with peptide concentration and no significant dimer product is observed in the absence of peptide. DPDPB-crosslinked products formed through disulfide-exchange reactions should be readily reversible by reduction as is seen for the covalently-linked EMP1-mediated dimer. Furthermore, we have constructed a covalently-linked dimeric form of EMP1 that demonstrates increased biological potency (Johnson et al, in preparation). The Cys<sup>181</sup> residues in D2 of the EBP dimer are 20.7 Å apart (Sγ-Sγ distance) which approximates the 16 Å length (and approximately 2 Å in bond length at each end) of the DPDPB crosslinker. Thus EMP1 mediates formation of a soluble EBP dimer complex in solution consistent with the crystal structure.

#### The WSXWS motif

The WSAWS sequence (residues 209-213) corresponding to the WSXWS box occurs in a β-bulge (Richardson, Adv. Prot. Chem. 34:167, 1981; Chan et al., Protein Science, 2:1574, 1993) immediately preceding β-strand G in D2. Residues in this motif do not interact with ligand, have no role in receptor-receptor interactions and are located on the opposite side of the receptor-receptor and receptor-ligand interface. The WSAWS box represents only a segment of a complex array of interactions that involves several other conserved side chains from the four-stranded β-sheet in D2. The indole ring systems of Trp<sup>209</sup> and Trp<sup>212</sup> point toward an external concave surface of the β-sheet and are only partially solvent exposed, whereas the Ala<sup>211</sup> side chain points directly out into solution. The amides and hydroxyls of both Ser<sup>210</sup> and Ser<sup>213</sup> form hydrogen bonds with the main

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chain of residues 198 and 196 of adjacent strand F in a pseudo  $\beta$ -sheet type interaction that resembles a modified wide  $\beta$ -bulge (Richardson, *Adv. Prot. Chem.* 34:167, 1981; Chan et al., *Protein Science*, 2:1574, 1993) where the sidechain hydroxyl rather than the carbonyl oxygen makes the  $\beta$ -sheet interaction. The  $\beta$ -bulge architecture places the two

5 Trp residues, which are spread four residues apart, on the same side of the  $\beta$ -sheet and not on opposite sides as in normal  $\beta$ -sheet or extended chain structures. The guanidinium group of Arg<sup>197</sup> from Strand F, the central residue (Richardson, *Adv. Prot. Chem.* 34: 167, 1981; Chan et al., *Protein Science*, 2:1574, 1993) in the bulge, is positioned exactly

10 between the two Trp indole rings to form an extended  $\pi$ -cation system (Kumpf et al., *Science* 261:1708, 1993. The center of the pyrrole ring of Trp<sup>209</sup>, the N $\epsilon$  of the Arg<sup>197</sup> and the center of the benzene ring of Trp<sup>212</sup> are positioned on a straight line with the three planes of the conjugated systems stacked parallel to each other at approximately 4 Å spacing. In addition, the aliphatic portion of the Arg<sup>199</sup> side chain has hydrophobic interactions with the indole ring of Trp<sup>209</sup>, completing the alternating stacking of two

15 aromatic and two positively-charged amino acid residues. The side chain of Glu<sup>157</sup> forms a hydrogen bond with Arg<sup>197</sup> presumably to help orient the guanidinium group and add some specificity and stabilization to the system.

It appears then that the linear WSXWS motif identified from sequence alignments of cytokine receptors represents only a component of a more complex conformational unit

20 that contributes a significant structural feature to D2. Aromatic residues have previously been suggested to have a stabilizing effect and play a role as a folding nuclei in structures of antiparallel  $\beta$ -sandwiches (Finkelstein et al., *Protein Eng.* 6:367, 1993). The amino-aromatic parallel stacking between the guanidinium group of arginine and the aromatic rings is a common feature in protein structures (Burley et al., *Adv. Prot. Chem.*, 39:125,

25 1988; Flocco et al., *J. Mol. Biol.*, 235:709, 1994), but a parallel triple stacking of  $\pi$ -cation systems is rare (Kim et al., *Biochemistry* 32:8465, 1993) although observed in other class-1 cytokine receptors, hGHbp and PRLR.



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The structural equivalents of the WSXWS motif in hGHbp (YGEFS) and PRLR (WSAWS) are involved in an even more intricate and complex array of  $\pi$ -cation interactions. The  $\pi$ -cation system is extended in hGHbp and PRLR to include an additional aromatic residue (Trp<sup>186</sup> for hGHbp and Trp<sup>156</sup> for PRLR) from the loop region that links  $\beta$ C and  $\beta$ C' in D2 and a positively-charged residue (Arg<sup>211</sup> for hGHbp and Arg<sup>147</sup> for PRLR) that stacks between the Trp and the second aromatic residue. The additional Arg residue is contributed either from the  $\beta$ F strand as in hGHbp (Arg<sup>211</sup>) or from  $\beta$ C as in PRLR (Arg<sup>147</sup>); the glutamine residue that hydrogen bonds and orients the arginine also switches strands. Sequence alignments suggest that this Arg-Gln switch could be common to other members of the class-1 cytokine receptor family. The extended  $\pi$ -cation system in hGHbp and PRLR consists of five positively charged and three aromatic residues stacked in an alternating order which comprises of Lys<sup>215</sup>, Tyr<sup>222</sup>, Arg<sup>213</sup>, Phe<sup>225</sup>, Arg<sup>211</sup>, Trp<sup>186</sup>, Lys<sup>179</sup> for hGHbp and Lys<sup>185</sup>, Trp<sup>191</sup>, Arg<sup>183</sup>, Trp<sup>194</sup>, Arg<sup>147</sup>, Trp<sup>156</sup>, Lys<sup>149</sup> for PRLR. The first aromatic-Arg-aromatic trio are approximately 4Å apart, as in EBP, but the second system is stacked closer together at approximately 3.6 Å spacings consistent with  $\pi$ - $\pi$  interaction (Burley et al., *Adv. Prot. Chem.*, 39:125, 1988; Flocco et al., *J. Mol. Biol.*, 235:709, 1994). The outer lysines also use the aliphatic portions of their side chains to form hydrophobic interactions with the aromatic rings. Based on sequence alignments with other members of the class-1 cytokine receptor superfamily, such structurally extended  $\pi$ -cation systems could exist in human thrombopietin, IL-6 and ciliary neurotrophic factor receptors, and in human IL-4 receptor based on structural modeling (Gustchina et al., *Proteins* 21:140, 1995). Although IFN- $\gamma$ R $\alpha$  and tissue factor do not have a WSXWS motif, the corresponding sequences TTEKS (residues 213-217) for IFN- $\gamma$ R $\alpha$  (Walter et al., *Nature* 376:230, 1995) and KSTDs (residues 201-205) for tissue factor (Muller et al., *Biochemistry* 33:10864, 1994; Harlos et al., *Nature* 370:662, 1994), maintain a very similar  $\beta$ -bulge. The consensus sequence among these five x-ray structures indicates that a serine or threonine in positions 2 and 5 maintain a common set of hydrogen bonds between their side chain hydroxyls and the mainchain of the neighboring strand. Only in hGHbp is there no hydroxyl-containing residue in position 2, but Ser<sup>226</sup> still maintains the equivalent interaction. A Ser<sup>226</sup> to Ala

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mutation abrogates hGHR binding to hGH, and its expression on the cell surface is drastically reduced (Baumgartner et al., *J. Biol. Chem.*, 269: 29094, 1994). In GM-CSFR $\alpha$  and IL-2R $\beta$ , point mutations of the serine residues cause a substantial decrease in cell surface expression but little or no effect on ligand binding (Ronco et al., *J. Biol. Chem.* 269:277, 1994; Miyazaki et al., *EMBO Journal* 10:3191, 1991).

Conservation of the WSXWS motif in EPOR or its equivalent in other members of the class 1 cytokine receptors has been proposed to be essential for biological activity and was thus assumed to be part of the receptor binding site (Yoshimura et al., *J. Biol. Chem.* 267:11619, 1992; Quelle, *Mol. Cell. Biol.* 12:4553 1992). For EPOR, a systematic study of 100 mutations of the WSAWS sequence demonstrates that most of the mutations of the two tryptophan and serine resulted in molecules that did not reach the cell surface but were retained in the endoplasmatic reticulum (Hilton et al., *Proc. Natl. Acad. Sci. USA* 92:190, 1995; Hilton et al., *J. Biol. Chem.* 271:4699, 1996). Furthermore, an Ala<sup>211</sup> to Glu mutation in the WSAWS sequence resulted in better transportation from the ER to the Golgi and a 3-5 fold increase of the number of EPOR molecules on the cell surface compared to the wild-type (Hilton et al., *Proc. Natl. Acad. Sci. USA* 92:190, 1995; Hilton et al., *J. Biol. Chem.* 271:4699, 1996). These results support our conclusion that the WSXWS sequence plays an important role in the structure and folding of D2 in EPOR and other related receptors.

## Comparison with other cytokine-receptor complex structures

The overall quaternary structure of the peptide-EBP complex substantially from the equivalent arrangement in the hGH-hGHR complex. The non-symmetric nature of the single four-helix-bundle structure of the growth hormone ligand results in an asymmetric homo-dimerization of the receptor that corresponds to a 159° rotation between receptors compared to the almost perfect 2-fold (180°) rotation for the EBP-peptide complex. The tertiary arrangement of domains within EBP and hGHbp is also somewhat different. When the equivalent EBP and hGHbp D2 domains are superimposed on each other, their corresponding D1 domains differ by a 12° rotation and a 4.3Å translation.

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The mechanism of hGH binding to its receptor has been well studied (Wells, Curr. Opin. Cell Biol. 6:163, 1994; Clackson et al., Science 267:383, 1995) and is sequential. Initial high affinity (nM) binding of the hormone with one receptor results in a buried surface of 1130 Å<sup>2</sup> on the receptor. The second hGHbp2 has a substantially smaller interface (deVos et al., Science 255:306, 1992) with the second binding site on hGH and interacts only with the preformed 1:1 complex to generate buried surface areas of 740 Å<sup>2</sup> with hGH and 440 Å<sup>2</sup> with the first hGHbp1 (deVos et al., Science 255:306, 1992; (Wells, Curr. Opin. Cell Biol. 6:163, 1994; Clackson et al., Science 267:383, 1995). The binding determinants of each hGHbp are comprised of the six recognition loops (L1-L6), three of which (L1-L3) come from one end of the β-sandwich structure in D1, one from the interdomain linker and two from D2.

Although these two receptor complexes, EBP-EMP1 and hGH-hGHbp, have different dimeric arrangements, which probably in this case represent differences in the size and shape of the natural versus synthetic ligand, both receptors share equivalent ligand recognition loops, L1, L3, L5 and L6 for the EBP and L1 to L6 for the hGHbp. A non-active PRLR, complexed with only one molecule of hGH, also uses the same contact loops (L1 to L6) (Somers et al., Nature 372:478, 1994). Based on similarity of the ligand recognition sites in hGHbp and PRLR, one would expect that the binding site of EBP, when its natural EPO ligand is bound, would extend to include two additional loops, L2 and L4, that comprise residues 59-63 (L2) between strands C to C', and residues 110-118 (L4) from the carboxyl end of βG in D1 and the interdomain linker. These six loops in EBP, hGHbp and PRLR are in structurally equivalent positions but vary in size, amino acid composition and conformation although the interacting portions of each loop (side or tip) remain similar; L1, L2, L3, L5 interact mainly with their tips and L6 with its side. In EBP, the L5 loop is three residues shorter than in hGHbp and PRLR, where the L6 loop is three and four residues longer than in hGHbp and PRLR, respectively. The L2 loop also varies (6 to 10 residues) among the three receptors but in EBP does not participate in peptide binding, and in hGHbp is partially disordered, although it does contact the hormone. In one respect, this situation is similar to the complementarity-

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determining regions (CDR's) in antibodies, where changes in length and sequence of the six binding loops impose specificity for different antigens, whereas the framework itself remains constant (Wilson et al., Ciba Foundation Symposium. Wiley, Chichester, 1991, Vol. 159, p. 13).

5 It has been shown for the hGH-hGHbp complex that only a subset of 9 out of 33 interacting residues that make up the structural epitope of the receptor constitute a functional epitope or hot spot (Wells, Curr. Opin. Cell Biol. 6:163, 1994; Clackson et al., Science 267:383, 1995) where high affinity binding interaction takes place. This reduced epitope is substantially smaller than the structural epitope and is comprised from residues  
10 (Arg<sup>43</sup>, Glu<sup>44</sup>, Ile<sup>103</sup>, Trp<sup>104</sup>, Ile<sup>105</sup>, Pro<sup>106</sup>, Asp<sup>163</sup>, and Trp<sup>169</sup>) which are located in contact loops L1, L3 and L5 with the most significant contribution (>4.5 kcal/mol) coming from two aromatic residues (Trp<sup>104</sup> and Trp<sup>169</sup>) in L3 and L5 (Wells, Curr. Opin. Cell Biol. 6:163, 1994; Clackson et al., Science 267:383, 1995; Wells, Proc. Natl Acad. Sci. USA 93:1, 1996). In EBP, Phe<sup>93</sup> is equivalent to Trp<sup>104</sup> in hGHbp, as suggested previously  
15 (Wells, Curr. Opin. Cell Biol. 6:163, 1994; Clackson et al., Science 267:383, 1995; Wells, Proc. Natl Acad. Sci. USA 93:1, 1996; Jolliffe et al., Nephrol. Dial. Trans. 10:suppl. 2, 28, 1995), but there is no homologous residue to Trp<sup>169</sup> in the shorter L5 loop. In the EBP-EMP1 complex, the Phe<sup>93</sup> peptide aromatic side chain occupies the equivalent position of the Trp<sup>169</sup> side chain in hGHbp. One can assume that when EPO binds to its  
20 receptor, the hormone may provide an aromatic residue to the hydrophobic core of the binding interface and/or the L6 loop in EBP may play a more significant role in the hormone binding than in hGHbp, since it is 3 residues longer and contains the aromatic Phe<sup>205</sup>.

25 In these three class-1 receptor structures, some loops are disordered which are in D2 for EBP for EBP (residues 164-166 in EBP1 and 133-135 in EBP2) and in D1 for both hGHbp (residues 55-58, 73-78 for hGHbp1 and 54-60, 73-75 for hGHbp2) and PRLR (residues 31-33, 84-86). Otherwise, these three class-1 cytokine receptors do not differ greatly in their over all tertiary structures; D1 and D2 have broadly similar general

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arrangement in all three receptors such that the angle between the long axes of the two domains is approximately 90 degrees. It is this arrangement of domains that allow these particular L1-L6 loops to be available for the recognition and binding of ligands. In a 2:2 complex between IFN- $\gamma$  and its class-2 receptor IFN- $\gamma$ R $\alpha$ , D1 and D2 are related by a 125 degree angle, which elongates the receptor and restricts the binding determinants that can be used for interaction with hormone; the L1 loop now becomes buried in the D1-D2 interface, although the other five loops (L2-L6) are still available for ligand interaction. This elongated interdomain arrangement is also observed in tissue factor (Muller et al., Biochemistry 33:10864, 1994; Harlos et al., Nature 370:662, 1994) which has a distant relationship to the cytokine receptor superfamily.

A mutational analysis of the EBP molecule indicates that the most crucial amino acid residue for binding EPO is Phe<sup>93</sup> in the L3 loop (Jolliffe et al., Nephrol. Dial. Trans. 10:suppl 2,28, 1995). The Phe93Ala mutant shows an increase in the IC<sub>50</sub> compared to the wild-type by a factor of approximately 1000, whereas other mutants (Ser91Ala, Ser92Ala, Val94Ala, Met150Ala and His153Ala) show small relative increases in the IC<sub>50</sub> of only 2.5-12.5 fold). The side chain of Phe<sup>93</sup> buries 66 Å<sup>2</sup> of molecular surface, which is the highest among interacting side chains. In hGHbp, the corresponding Trp104Ala mutation results in an increase in the K<sub>d</sub> by a factor of more than 2,500 compared to the wild-type indicating the equivalent importance of this residue in hGH binding and its key contribution to the hydrophobic core of the functional epitope (Wells, Curr. Opin. Cell Biol. 6:163, 1994; Clackson et al., Science 267:383, 1995; Bass et al. Proc. Natl. Acad. Sci. USA 88:4498, 1991).

#### **The role of dimerization on signal transduction**

In the EBP-EMP1 complex structure, we surprisingly observe that a peptide, unrelated in sequence and probably in structure, to the natural ligand, can induce a biologically active dimerization of EPO receptor that promotes signal transduction and cell proliferation. Comparison of three class-1 cytokine receptor complexes, whose structures have been determined so far, suggests that when the natural EPO hormone, which is

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proposed to have a structure of a four-helix bundle (Boissel et al., J. Biol. Chem. 268:15983, 1993), induces receptor dimerization, it is more likely to resemble the hGH-hGHbp assemblage. This would suggest that more than one mode of productive extracellular dimerization is permissive for intracellular dimerization of the cytoplasmic domains with two JAK2 molecules in order to initialize the cascade of events that produces the biologically relevant signal (Thle et al., Seminars in Immunology 5:375, 1993; Klingmuller et al., Cell 80:729, 1995). The peptide-EBP structure would then represent only one possible dimeric arrangement that promotes signal transduction.

Mutant EPOR molecules, containing a single Arg to Cys mutation (Arg<sup>130</sup> in human and Arg<sup>129</sup> in murine), have been shown to form biologically active dimers in the absence of EPO (Yoshimura et al., J. Biol. Chem. 267:11619, 1992; Watowich et al., Proc. Natl. Acad. Sci. USA 89:2140, 1992; Watowich et al., Mol. Cell. Biol. 14:3535, 1994), suggesting that extracellular receptor homo-dimerization may be sufficient in itself for signal transduction. It has been shown in another system (Spencer et al., Science 262:1019, 1993) that activation of a specific set of transcription factors can be induced by the chemical crosslinking of cytoplasmic domains of modified cell membrane receptors that do not contain the extracellular and transmembrane domains. These receptors are not related to the cytokine receptor superfamily but illustrate that oligomerization plays a key role in activation of the receptor, and that the main functional role of the extracellular, ligand-binding domain is to allow (in the presence of ligand) dimerization or oligomerization and induce similar association of the cytoplasmic domains.

Mutagenesis experiments originally suggested a role for the WSXWS motif in this cell signalling process (Yoshimura et al., J. Biol. Chem. 267:11619, 1992; Quelle et al. Mol. Cell. Biol. 12:4553, 1992; Chiba et al., Biochem. Biophys. Res. Comm. 184:485, 1992) possibly by promoting receptor homo-dimerization. However, truncation mutants of EPOR (Miura et al., Arch. Biochem. Biophys. 306:200, 1993) do not confirm this role for the WSXWS motif. The EBP-EMP1 complex structure shows that the WSXWS motif

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of the EPOR, as for the hGH-hGHbp complex (deVos et al., Science 255:306, 1992) is located on the opposite face of the molecule from the receptor dimerization. In the absence of unliganded structures for the extracellular domains of EPOR, hGHR and PRLR, it is not possible to determine whether any conformation change occurs on ligand binding that would involve the WSXWS box. Apart from being a striking structural feature in D2, and its obvious proximity to the membrane spanning domain, one cannot rule out possible interactions of this region with some other cell surface molecules that are involved somehow in the signal transduction process.

#### **Towards design of small molecule mimetics**

The structure of the EMP1 dimer demonstrates that a peptide considerably smaller than the natural hormone can act as an agonist and induce the appropriate biological response. The peptide can be assumed to form a substantially smaller contact interface than the natural hormone with the receptor. The peptide binding site in EBP forms an almost flat surface, which is mainly hydrophobic in nature, without any cavities or charged residues that are normally essential for the specific targeting of small molecule ligands to a receptor binding site. The hGHbp study (Wells et al., Science 267:383, 1995; Wells, Proc. Natl. Acad. Sci. USA 93:1, 1996) shows that only a small part of the observed structural binding site, the so-called functional epitope (*supra*), contributes most of the binding energy and strongly implied that a "minimized" hormone designed to interact with this site could form sufficient interactions to activate the receptor. Furthermore, the limited site of interaction of the small agonist peptide with the EBP corresponds almost exactly to the smaller functional epitope derived from alanine scanning of hGH and hGHbp. Thus, by a different approach, we have arrived at the similar conclusion that a small number of key interactions can contribute to a functional epitope on a receptor. Understanding of this simplified interaction surface can be now combined with further mutational studies to assist in identifying the most crucial residues in the functional epitope, and consequently provide a more practical target for drug design.

#### **Data Collection, MIR and Refinement Statistics**

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The crystallographic data is summarized in Table 1. Native crystallographic data were collected on a Siemens multiwire area detector mounted on an Elliott GX-18 generator, operating at 40kV and 55mA, with a crystal-to-detector distance of 120mm. Two derivative data sets were collected on a MAR image plate mounted on a Siemens generator operating at 50kV and 80mA, with crystal-to-image plate distance of 150mm. Data were integrated, scaled and reduced using the programs XENGEN (Howard et al., J. App. Cryst. 20:383, 1987) for the native data and DENZO/SCALEPACK (Otwinowski et al., SERC Daresbury Laboratory, Warrington, 1993) for the derivative data. Initial multiple isomorphous replacement anomalous scattering (MIRAS) phases were calculated to 3.1 Å using the program package PHASES (Furey, American Crystallographic Association Fortieth Anniversary Meeting, New Orleans, LA, 1990) with a mean figure of merit of 0.64 (25.0-3.1 Å). Phases were refined in PHASES using the solvent flattening protocol to a mean figure of merit of 0.92 (25.0-3.1 Å). The quality of the map was generally good and most of the complex structure (94%) could be fitted using the graphics program O (Jones et al., Acta Crystallogr A47:110, 1991). The register of the amino acid residues was verified from the positions of the two disulfide bridges in D1, and the positions of the two Hg's from the mercury acetate derivative that were correctly assumed to bind to the free Cys<sup>181</sup> residue. the peptide interpretation was verified from another data set from a complex between EBP and an iodinated peptide (Tyr<sup>P4</sup> was substituted for *p*-iodo-Phe), which diffracted to 3.3Å resolution, that in difference Fourier ( $F_{\text{iodo}} - F_{\text{free}}$ ) $\alpha_{\text{MIRAS}}$  gave a clear indication of the location of the iodine atoms. The structure was refined using the slow-cooling protocol in X-PLOR 3.1 (Brunger et al., Acta Crystallogr A46:585, 1990; Brunger, X-PLOR, Version 3.1: A System for X-ray and NMR, Yale Univ. Press, New Haven, CT, 1992) and rebuilt using Fo-Fc, 3Fo-2Fc and SIGMAA (Read, Acta Crystallogr. A42:140, 1986) weighted electron density maps. After every two cycles of refinement, a set of simulated annealing omit maps (7-10%) to reduce model bias was calculated and the entire structure rebuilt. After several cycles of refinement, individual temperature factors were calculated and after 10 cycles of refinement and model building, the R-value was 0.21 for 8.0-2.8 Å data with  $F > 1\sigma$  (13,984 reflections). The average thermal parameters for receptor I, receptor II and the



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peptides are  $10.5\text{\AA}^2$ ,  $12.3\text{\AA}$  and  $10.7\text{\AA}$  respectively. Only one non-glycine residue [Asn<sup>164</sup> in EBP2], located in a loop region in D1, is in a disallowed region in the Ramachandran plot. No solvent molecules were included in the model due to the moderate resolution ( $2.8\text{\AA}$ ) of the structure determination.

5     **Binding Contacts**

Binding contacts are summarized, in part, in Table 2: Hydrogen bond interactions in the binding site of the EBP-EMP1 complex. Due to the symmetrical nature of the complex, peptide-1 and peptide-2 have equivalent interactions with the two EBP molecules. The hydrogen bond interactions were analyzed using HBPLUS (McDonald et al., J. Mol. Biol.  
10     238:777, 1994), based upon both distance ( $3.9\text{\AA}$  cutoff) and geometrical considerations.

A number of embodiments of the present invention have been described. Nevertheless, it will be understood that various modifications may be made without departing from the spirit and scope of the invention. Accordingly, it is to be understood that the invention is not to be limited by the specific illustrated embodiment, but only by the scope of the  
15     appended claims.

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## EBP1-PEPTIDE1

VDW	1	LEU	33	CB	4	PHE	308	CE1	1	3.95
VDW	1	LEU	33	CB	4	PHE	308	CD1	1	4.11
VDW	1	PHE	93	CE1	4	TRP	313	CH2	1	3.74
VDW	1	PHE	93	CZ	4	TRP	313	CH2	1	3.98
VDW	1	PHE	93	CZ	4	TRP	313	CZ2	1	4.08
VDW	1	PRO	149	CA	4	GLY	309	O	1	3.59
VDW	1	PRO	149	CB	4	GLY	309	O	1	3.49
VDW	1	PRO	149	C	4	GLY	309	O	1	3.66
VDW	1	MET	150	N	4	PRO	310	O	1	3.35
VDW	1	MET	150	N	4	PRO	310	C	1	3.62
VDW	1	MET	150	CA	4	LEU	311	O	1	3.41
VDW	1	MET	150	CA	4	GLY	309	O	1	3.78
VDW	1	MET	150	CA	4	LEU	311	C	1	3.87
VDW	1	MET	150	CG	4	PHE	308	CD2	1	3.50
VDW	1	MET	150	CG	4	PHE	308	CB	1	3.70
VDW	1	MET	150	CG	4	PHE	308	CG	1	3.79
VDW	1	MET	150	SD	4	PHE	308	CD2	1	3.52
VDW	1	MET	150	SD	4	THR	312	C	1	3.55
VDW	1	MET	150	SD	4	THR	312	CA	1	3.58
VDW	1	MET	150	SD	4	TRP	313	N	1	3.75
VDW	1	MET	150	SD	4	PHE	308	CA	1	3.91
VDW	1	MET	150	SD	4	PHE	308	CB	1	4.03
VDW	1	MET	150	CE	4	PHE	308	CD2	1	3.45
VDW	1	MET	150	CE	4	TRP	313	CE2	1	3.71
VDW	1	MET	150	CE	4	PHE	308	CE2	1	3.79
VDW	1	MET	150	CE	4	TRP	313	CD2	1	3.83
VDW	1	MET	150	CE	4	TRP	313	NE1	1	3.91
VDW	1	MET	150	CE	4	TRP	313	CZ2	1	4.10
VDW	1	MET	150	C	4	LEU	311	O	1	3.41
VDW	1	THR	151	N	4	LEU	311	O	1	3.45
VDW	1	THR	151	CA	4	PRO	310	O	1	3.82
VDW	1	THR	151	CB	4	PRO	310	O	1	3.56
VDW	1	THR	151	OG1	4	LEU	311	CD2	1	3.43
VDW	1	THR	151	OG1	4	LEU	311	CA	1	3.91
VDW	1	THR	151	CG2	4	PRO	310	O	1	3.60
VDW	1	SER	152	CB	4	LEU	311	O	1	3.54
VDW	1	HIS	153	ND1	4	LEU	311	O	1	3.57
SHORTVDW	1	HIS	153	CE1	4	THR	312	OG1	1	2.87
VDW	1	HIS	153	CE1	4	THR	312	CB	1	3.48
VDW	1	HIS	153	CE1	4	THR	312	CA	1	3.76
VDW	1	HIS	153	NE2	4	THR	312	OG1	1	3.57
VDW	1	PHE	205	CE2	4	PHE	308	CZ	1	3.90
VDW	1	PHE	205	CZ	4	PHE	308	CE2	1	3.40
VDW	1	PHE	205	CZ	4	PHE	308	CZ	1	3.53

## EBP2-PEP1

VDW	2	SER	591	CA	4	TYR	304	OH	1	3.44
VDW	2	SER	591	CB	4	TYR	304	OH	1	3.88
VDW	2	SER	591	CB	4	PRO	317	CB	1	3.95
VDW	2	SER	591	OG	4	TYR	304	OH	1	3.44
VDW	2	SER	591	OG	4	PRO	317	CB	1	3.61
VDW	2	SER	591	OG	4	TYR	304	CZ	1	3.83
VDW	2	SER	591	OG	4	TYR	304	CE2	1	3.84
VDW	2	SER	591	C	4	TYR	304	OH	1	3.62
VDW	2	SER	592	N	4	TYR	304	CE2	1	3.66
VDW	2	SER	592	N	4	TYR	304	CZ	1	3.68
VDW	2	SER	592	CA	4	TYR	304	OH	1	3.80
VDW	2	SER	592	CB	4	TYR	304	OH	1	3.73
VDW	2	SER	592	C	4	TYR	304	CE2	1	4.00
VDW	2	SER	592	O	4	TYR	304	CE2	1	3.53
VDW	2	SER	592	O	4	PRO	317	CD	1	3.59
VDW	2	PHE	593	CB	4	CYS	315	O	1	3.74
VDW	2	PHE	593	CD1	4	CYS	315	CB	1	3.55
VDW	2	PHE	593	CD1	4	TYR	304	CD2	1	3.72

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VDW	2 PHE 593	CD1	4 TYR 304	CE2	1	3.90
VDW	2 PHE 593	CE1	4 CYS 315	CB	1	3.71
SHORTVDW	2 VAL 594	CG1	4 PRO 317	CG	1	3.17
SHORTVDW	2 VAL 594	CG1	4 PRO 317	CD	1	3.23
EBP1-PEPTIDE2						
VDW	1 SER 91	CB	4 PRO 417	CB	1	3.84
VDW	1 SER 91	CB	4 PRO 417	CG	1	3.90
VDW	1 SER 91	OG	4 PRO 417	CB	1	3.90
VDW	1 SER 92	N	4 TYR 404	CE2	1	3.82
VDW	1 SER 92	CA	4 TYR 404	OH	1	3.85
VDW	1 SER 92	CB	4 TYR 404	OH	1	3.42
VDW	1 SER 92	CB	4 TYR 404	CZ	1	4.04
VDW	1 SER 92	CB	4 TYR 404	CE2	1	4.09
VDW	1 PHE 93	CB	4 CYS 415	O	1	3.43
VDW	1 PHE 93	CD1	4 TYR 404	CE2	1	3.71
VDW	1 PHE 93	CD1	4 TYR 404	CD2	1	3.83
VDW	1 PHE 93	CD1	4 CYS 415	CB	1	3.92
VDW	1 PHE 93	CE1	4 CYS 415	CB	1	4.08
VDW	1 PHE 93	CE1	4 TYR 404	CE2	1	4.09
VDW	1 VAL 94	CG1	4 PRO 417	CG	1	3.54
VDW	1 VAL 94	CG1	4 PRO 417	CD	1	3.54
VDW	1 VAL 94	CG2	4 PRO 417	CG	1	4.11
EBP2-PEPTIDE2						
SHORTVDW	2 LEU 533	CB	4 PHE 408	CE1	1	3.14
VDW	2 LEU 533	CB	4 PHE 408	CD1	1	3.77
VDW	2 LEU 533	CB	4 PHE 408	CZ	1	4.00
VDW	2 LEU 533	CG	4 PHE 408	CE1	1	4.05
VDW	2 LEU 533	CD1	4 PHE 408	CE1	1	3.75
VDW	2 LEU 533	CD1	4 PHE 408	CZ	1	3.92
VDW	2 LEU 533	O	4 PHE 408	CE1	1	3.67
VDW	2 PHE 593	CE1	4 TRP 413	CH2	1	3.34
VDW	2 PHE 593	CE1	4 TRP 413	CZ2	1	3.41
VDW	2 PHE 593	CZ	4 TRP 413	CZ2	1	3.67
VDW	2 PHE 593	CZ	4 TRP 413	CH2	1	3.96
VDW	2 PRO 649	CA	4 GLY 409	O	1	3.79
VDW	2 PRO 649	CB	4 GLY 409	O	1	3.56
VDW	2 PRO 649	C	4 PRO 410	O	1	3.72
VDW	2 MET 650	CA	4 PRO 410	O	1	3.59
VDW	2 MET 650	CA	4 GLY 409	O	1	3.67
VDW	2 MET 650	CA	4 LEU 411	O	1	3.77
VDW	2 MET 650	CG	4 PHE 408	CD2	1	3.80
VDW	2 MET 650	CG	4 PHE 408	CG	1	3.92
VDW	2 MET 650	CG	4 PHE 408	CB	1	4.05
VDW	2 MET 650	SD	4 TRP 413	N	1	3.72
VDW	2 MET 650	SD	4 THR 412	C	1	3.75
VDW	2 MET 650	SD	4 PHE 408	CD2	1	3.76
VDW	2 MET 650	SD	4 THR 412	CA	1	3.78
VDW	2 MET 650	SD	4 PHE 408	CA	1	4.02
VDW	2 MET 650	CE	4 TRP 413	CE2	1	3.67
VDW	2 MET 650	CE	4 TRP 413	NE1	1	3.76
VDW	2 MET 650	CE	4 TRP 413	CD2	1	3.76
VDW	2 MET 650	CE	4 PHE 408	CD2	1	3.83
VDW	2 MET 650	CE	4 TRP 413	CD1	1	3.88
VDW	2 MET 650	CE	4 TRP 413	N	1	3.89
VDW	2 MET 650	CE	4 TRP 413	CG	1	3.90
VDW	2 MET 650	C	4 LEU 411	O	1	3.54
VDW	2 MET 650	C	4 PRO 410	O	1	3.57
VDW	2 THR 651	N	4 LEU 411	O	1	3.56
VDW	2 THR 651	N	4 PRO 410	C	1	3.77
VDW	2 THR 651	CA	4 PRO 410	O	1	3.41
SHORTVDW	2 THR 651	CB	4 PRO 410	O	1	3.03
VDW	2 THR 651	CB	4 PRO 410	C	1	3.98
VDW	2 THR 651	CB	4 LEU 411	CA	1	4.02
VDW	2 THR 651	OG1	4 PRO 410	C	1	3.62

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VDW	2	SER	652	N	4	LEU	411	C	1	3.83
VDW	2	SER	652	CA	4	LEU	411	O	1	3.51
VDW	2	SER	652	CB	4	LEU	411	O	1	3.18
VDW	2	SER	652	CB	4	LEU	411	C	1	4.09
VDW	2	SER	652	OG	4	THR	412	CB	1	3.73
SHORTVDW	2	HIS	653	CE1	4	THR	412	OG1	1	3.00
VDW	2	HIS	653	CE1	4	THR	412	CB	1	3.91
PEPTIDE1-PEPTIDE2										
SHORTVDW	3	THR	303	OG1	4	HIS	407	CB	1	2.94
VDW	3	THR	303	OG1	4	HIS	407	CA	1	3.61
VDW	3	TYR	304	CB	4	CYS	406	O	1	3.86
VDW	3	TYR	304	CD1	4	TRP	413	CZ3	1	3.81
VDW	3	TYR	304	CD1	4	TRP	413	CH2	1	3.94
VDW	3	TYR	304	O	4	CYS	406	N	1	3.33
VDW	3	TYR	304	O	4	CYS	406	O	1	3.47
VDW	3	TYR	304	O	4	SER	405	CA	1	3.57
VDW	3	SER	305	CA	4	TYR	404	O	1	3.51
VDW	3	SER	305	C	4	TYR	404	O	1	3.77
VDW	3	CYS	306	O	4	THR	403	CB	1	3.50
VDW	3	CYS	306	O	4	TYR	404	CB	1	3.54
VDW	3	CYS	306	O	4	TYR	404	CD1	1	3.59
VDW	3	CYS	306	O	4	TYR	404	CA	1	3.75
VDW	3	CYS	306	CB	4	CYS	406	SG	1	3.81
VDW	3	CYS	306	SG	4	CYS	406	SG	1	3.75
VDW	3	CYS	306	SG	4	CYS	406	CB	1	4.06
VDW	3	PHE	308	CE1	4	TYR	404	OH	1	3.93
VDW	3	PHE	308	CE1	4	TYR	404	CE1	1	4.08
VDW	3	TRP	313	CG	4	TRP	413	CD1	1	3.85
SHORTVDW	3	TRP	313	CD1	4	TRP	413	CD1	1	3.04
VDW	3	TRP	313	CD1	4	TRP	413	NE1	1	3.37
VDW	3	TRP	313	CD1	4	TRP	413	CG	1	4.09
VDW	3	TRP	313	NE1	4	TRP	413	CD1	1	3.31
VDW	3	TRP	313	CZ2	4	CYS	415	SG	1	3.84
VDW	3	TRP	313	CH2	4	CYS	415	SG	1	3.83
VDW	3	CYS	315	SG	4	TRP	413	CZ2	1	3.59
VDW	3	CYS	315	SG	4	TRP	413	CE2	1	3.95
VDW	3	CYS	315	SG	4	TRP	413	CH2	1	4.00
VDW	3	GLN	318	CD	4	GLN	418	NE2	1	3.28
VDW	3	GLN	318	OE1	4	SER	405	CB	1	3.80

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REMARK THE COMPLEX BETWEEN THE EXTRACELLULAR DOMAIN OF ERYTHROPOIETIC  
 REMARK RECEPTOR (EBP) AND AN AGONIST EPO MIMETIC PEPTIDE: 1 (EMF1)  
 REMARK \*\*\*\*\* WARNING \*\*\*\*\* RESIDUES 21-23 (521-522) and 164-166, 633-634  
 REMARK HAVE WEAK OR NO ELECTRON DENSITY MAP AND HAVE BEEN MODELED  
 REMARK INTO THE STRUCTURE. THESE RESIDUES HAVE A HIGH B OF 90.

REMARK THE STRUCTURE CONSISTS OF TWO RECEPTOR (RESIDUES 10-220, 510-720)  
 REMARK AND PEPTIDE (RESIDUES 303-318, 403-418) MOLECULES.

ATOM	1	N	LYS	10	40.090	29.257	22.042	1.00	22.57
ATOM	2	CA	LYS	10	39.634	30.133	20.962	1.00	23.45
ATOM	3	CB	LYS	10	38.753	29.361	19.979	1.00	22.87
ATOM	4	CG	LYS	10	38.334	30.155	18.735	1.00	22.92
ATOM	5	CD	LYS	10	38.119	29.212	17.552	1.00	24.27
ATOM	6	CE	LYS	10	37.165	28.015	17.890	1.00	26.55
ATOM	7	NZ	LYS	10	35.685	28.367	17.998	1.00	26.18
ATOM	8	C	LYS	10	38.921	31.427	21.420	1.00	22.91
ATOM	9	O	LYS	10	39.589	32.442	21.636	1.00	24.17
ATOM	10	N	PHE	11	37.602	31.386	21.640	1.00	21.40
ATOM	11	CA	PHE	11	36.868	32.588	22.026	1.00	18.56
ATOM	12	CB	PHE	11	35.549	32.257	22.725	1.00	19.07
ATOM	13	CG	PHE	11	34.497	33.362	22.609	1.00	20.24
ATOM	14	CD1	PHE	11	34.862	34.717	22.670	1.00	19.49
ATOM	15	CD2	PHE	11	33.142	33.038	22.400	1.00	19.51
ATOM	16	CE1	PHE	11	33.910	35.728	22.527	1.00	19.64
ATOM	17	CE2	PHE	11	32.180	34.041	22.257	1.00	20.10
ATOM	18	CZ	PHE	11	32.566	35.395	22.321	1.00	19.48
ATOM	19	C	PHE	11	37.644	33.567	22.887	1.00	19.32
ATOM	20	O	PHE	11	37.776	34.740	22.516	1.00	18.89
ATOM	21	N	GLU	12	38.181	33.106	24.016	1.00	20.71
ATOM	22	CA	GLU	12	38.905	34.036	24.886	1.00	20.59
ATOM	23	CB	GLU	12	39.253	33.423	26.246	1.00	21.48
ATOM	24	CG	GLU	12	40.185	34.309	27.123	1.00	23.60
ATOM	25	CD	GLU	12	39.455	35.301	28.056	1.00	25.09
ATOM	26	OE1	GLU	12	40.024	36.417	28.275	1.00	23.07
ATOM	27	OE2	GLU	12	38.356	34.952	28.589	1.00	21.05
ATOM	28	C	GLU	12	40.137	34.539	24.172	1.00	19.22
ATOM	29	O	GLU	12	40.513	35.703	24.334	1.00	18.49
ATOM	30	N	SER	13	40.730	33.687	23.341	1.00	17.67
ATOM	31	CA	SER	13	41.903	34.094	22.571	1.00	16.71
ATOM	32	CB	SER	13	42.522	32.898	21.851	1.00	18.51
ATOM	33	OG	SER	13	42.256	32.959	20.459	1.00	23.19
ATOM	34	C	SER	13	41.570	35.202	21.554	1.00	15.57
ATOM	35	O	SER	13	42.239	36.248	21.546	1.00	15.13
ATOM	36	N	LYS	14	40.563	34.955	20.698	1.00	12.00
ATOM	37	CA	LYS	14	40.117	33.912	19.675	1.00	8.51
ATOM	38	CB	LYS	14	39.062	35.287	18.769	1.00	5.06
ATOM	39	CG	LYS	14	39.629	34.366	17.714	1.00	2.36
ATOM	40	CD	LYS	14	38.566	33.862	15.761	1.00	2.00
ATOM	41	CE	LYS	14	39.191	33.270	15.496	1.00	2.27
ATOM	42	NZ	LYS	14	38.193	32.742	14.528	1.00	2.00
ATOM	43	C	LYS	14	39.586	37.198	20.295	1.00	9.05
ATOM	44	O	LYS	14	39.782	38.290	19.755	1.00	7.15
ATOM	45	N	ALA	15	38.920	37.053	21.442	1.00	11.98
ATOM	46	CA	ALA	15	38.375	38.188	22.194	1.00	12.13
ATOM	47	CB	ALA	15	37.571	37.697	23.378	1.00	11.49
ATOM	48	C	ALA	15	39.592	38.960	22.666	1.00	12.49
ATOM	49	O	ALA	15	39.683	40.189	22.535	1.00	13.58
ATOM	50	N	ALA	16	40.560	38.207	23.167	1.00	13.97
ATOM	51	CA	ALA	16	41.792	38.796	23.615	1.00	14.97
ATOM	52	CB	ALA	16	42.771	37.710	24.052	1.00	14.76
ATOM	53	C	ALA	16	42.361	39.567	22.426	1.00	15.45
ATOM	54	O	ALA	16	42.624	40.759	22.937	1.00	15.35
ATOM	55	N	LEU	17	42.444	38.896	21.274	1.00	16.12
ATOM	56	CA	LEU	17	43.007	39.467	20.042	1.00	15.92
ATOM	57	CB	LEU	17	43.012	39.428	18.910	1.00	15.72
ATOM	58	CG	LEU	17	44.204	37.485	18.662	1.00	17.46
ATOM	59	CD1	LEU	17	45.474	38.294	18.506	1.00	16.45
ATOM	60	CD2	LEU	17	44.360	36.462	19.774	1.00	16.32
ATOM	61	C	LEU	17	42.374	40.741	19.512	1.00	15.04
ATOM	62	O	LEU	17	42.985	41.438	18.711	1.00	15.91
ATOM	63	N	LEU	18	41.136	41.018	19.908	1.00	17.34
ATOM	64	CA	LEU	18	40.434	42.210	19.443	1.00	15.72
ATOM	65	CB	LEU	18	38.995	41.867	19.022	1.00	13.72
ATOM	66	CG	LEU	18	38.725	41.263	17.640	1.00	9.76
ATOM	67	CD1	LEU	18	37.235	41.260	17.329	1.00	5.61
ATOM	68	CD2	LEU	18	39.422	42.117	16.625	1.00	10.13
ATOM	69	C	LEU	18	40.393	43.284	20.500	1.00	17.38
ATOM	70	O	LEU	18	39.876	44.375	20.257	1.00	19.32

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ATOM	71	N	ALA	19	40.921	42.981	21.680	1.00	19.88	7
ATOM	72	CA	ALA	19	40.925	43.941	22.789	1.00	22.64	6
ATOM	73	CB	ALA	19	41.560	43.331	24.041	1.00	22.75	6
ATOM	74	C	ALA	19	41.601	45.273	22.445	1.00	25.13	6
ATOM	75	O	ALA	19	42.026	45.499	21.294	1.00	25.03	3
ATOM	76	N	ALA	20	41.649	46.164	23.453	1.00	28.77	7
ATOM	77	CA	ALA	20	42.246	47.514	23.323	1.00	28.51	6
ATOM	78	CB	ALA	20	41.529	48.505	24.310	1.00	28.93	6
ATOM	79	C	ALA	20	43.770	47.526	23.562	1.00	27.54	6
ATOM	80	O	ALA	20	44.438	46.484	23.505	1.00	27.85	3
ATOM	81	N	ARG	21	44.326	48.699	23.848	1.00	90.00	7
ATOM	82	CA	ARG	21	45.765	48.784	24.075	1.00	90.00	6
ATOM	83	CB	ARG	21	46.562	48.353	22.819	1.00	90.00	6
ATOM	84	CG	ARG	21	45.827	48.428	21.446	1.00	90.00	6
ATOM	85	CD	ARG	21	45.719	49.838	20.863	1.00	90.00	6
ATOM	86	NE	ARG	21	44.765	50.675	21.591	1.00	90.00	7
ATOM	87	CZ	ARG	21	43.448	50.471	21.610	1.00	90.00	6
ATOM	88	NH1	ARG	21	42.915	49.448	20.926	1.00	90.00	7
ATOM	89	NH2	ARG	21	42.669	51.270	22.350	1.00	90.00	7
ATOM	90	C	ARG	21	46.298	50.118	24.590	1.00	90.00	5
ATOM	91	O	ARG	21	45.875	51.199	24.132	1.00	90.00	8
ATOM	92	N	GLY	22	47.158	50.016	25.614	1.00	90.00	7
ATOM	93	CA	GLY	22	47.824	51.171	26.193	1.00	90.00	5
ATOM	94	C	GLY	22	49.053	51.371	25.314	1.00	90.00	6
ATOM	95	O	GLY	22	48.939	51.174	24.089	1.00	90.00	3
ATOM	96	N	PRO	23	50.230	51.765	25.872	1.00	90.00	7
ATOM	97	CD	PRO	23	50.318	52.564	27.119	1.00	90.00	5
ATOM	98	CA	PRO	23	51.451	51.971	25.062	1.00	90.00	5
ATOM	99	CB	PRO	23	51.713	53.452	25.287	1.00	90.00	5
ATOM	100	CG	PRO	23	51.527	53.517	26.850	1.00	90.00	5
ATOM	101	C	PRO	23	52.681	51.167	25.544	1.00	90.00	5
ATOM	102	O	PRO	23	52.560	50.067	26.123	1.00	90.00	3
ATOM	103	N	GLU	24	53.863	51.758	25.308	1.00	28.27	7
ATOM	104	CA	GLU	24	55.136	51.178	25.741	1.00	24.32	6
ATOM	105	CB	GLU	24	56.332	52.009	25.238	1.00	24.01	6
ATOM	106	CG	GLU	24	56.479	52.149	23.723	1.00	25.03	6
ATOM	107	CD	GLU	24	56.710	50.822	22.959	1.00	24.22	6
ATOM	108	OE1	GLU	24	57.171	50.954	21.793	1.00	23.14	3
ATOM	109	OE2	GLU	24	56.430	49.692	23.478	1.00	18.50	3
ATOM	110	C	GLU	24	55.117	51.264	27.268	1.00	23.39	5
ATOM	111	O	GLU	24	54.874	52.365	27.829	1.00	24.36	3
ATOM	112	N	GLU	25	55.342	50.124	27.925	1.00	18.35	7
ATOM	113	CA	GLU	25	55.371	50.058	29.377	1.00	14.09	5
ATOM	114	CB	GLU	25	53.962	49.818	29.907	1.00	17.09	5
ATOM	115	CG	GLU	25	53.789	49.985	31.410	1.00	22.21	5
ATOM	116	CD	GLU	25	53.199	51.348	31.799	1.00	27.17	5
ATOM	117	OE1	GLU	25	53.461	52.355	31.057	1.00	27.15	3
ATOM	118	OE2	GLU	25	52.461	51.401	32.837	1.00	26.11	3
ATOM	119	C	GLU	25	56.249	48.872	29.725	1.00	11.99	5
ATOM	120	O	GLU	25	56.056	47.779	29.181	1.00	14.38	3
ATOM	121	N	LEU	26	57.246	49.098	30.572	1.00	8.48	7
ATOM	122	CA	LEU	26	58.147	48.034	31.001	1.00	5.93	5
ATOM	123	CB	LEU	26	59.395	48.624	31.652	1.00	4.03	5
ATOM	124	CG	LEU	26	60.719	47.880	31.488	1.00	2.00	5
ATOM	125	CD1	LEU	26	61.537	48.145	32.704	1.00	4.41	5
ATOM	126	CD2	LEU	26	60.535	46.401	31.317	1.00	2.00	5
ATOM	127	C	LEU	26	57.409	47.188	32.030	1.00	6.68	5
ATOM	128	O	LEU	26	56.951	47.727	33.041	1.00	9.43	3
ATOM	129	N	LEU	27	57.310	45.880	31.797	1.00	5.17	7
ATOM	130	CA	LEU	27	56.613	44.996	32.719	1.00	5.71	5
ATOM	131	CB	LEU	27	55.428	44.334	32.035	1.00	6.50	5
ATOM	132	CG	LEU	27	54.281	45.268	31.673	1.00	10.84	5
ATOM	133	CD1	LEU	27	53.101	44.428	31.125	1.00	10.81	5
ATOM	134	CD2	LEU	27	53.871	46.130	32.906	1.00	7.08	5
ATOM	135	C	LEU	27	57.454	43.923	33.397	1.00	7.41	5
ATOM	136	O	LEU	27	58.003	43.037	32.742	1.00	7.62	3
ATOM	137	N	CYS	28	57.460	43.964	34.726	1.00	7.42	7
ATOM	138	CA	CYS	28	58.208	43.027	35.554	1.00	4.67	5
ATOM	139	C	CYS	28	57.246	42.359	36.529	1.00	4.38	5
ATOM	140	O	CYS	28	56.217	42.945	36.861	1.00	2.56	5
ATOM	141	CB	CYS	28	59.266	43.791	36.357	1.00	3.64	5
ATOM	142	SG	CYS	28	60.429	44.763	35.358	1.00	4.87	16
ATOM	143	N	PHE	29	57.595	41.155	36.977	1.00	2.00	7
ATOM	144	CA	PHE	29	56.817	40.403	37.943	1.00	2.00	5
ATOM	145	CB	PHE	29	55.474	39.899	37.322	1.00	4.36	5
ATOM	146	CG	PHE	29	55.586	38.643	36.437	1.00	3.43	5
ATOM	147	CD1	PHE	29	55.493	37.369	36.990	1.00	2.00	5
ATOM	148	CD2	PHE	29	55.790	38.747	35.058	1.00	2.00	5

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ATOM	149	CE1 PHE	29	55.605	36.243	36.206	1.00	2.00
ATOM	150	CE2 PHE	29	55.906	37.616	34.266	1.00	2.00
ATOM	151	CZ PHE	29	55.815	36.365	34.843	1.00	2.00
ATOM	152	C PHE	29	57.678	39.260	38.543	1.00	3.80
ATOM	153	O PHE	29	58.702	38.897	37.957	1.00	2.00
ATOM	154	N THR	30	57.340	38.814	39.766	1.00	4.17
ATOM	155	CA THP	30	58.021	37.694	40.463	1.00	3.12
ATOM	156	CB THP	30	58.720	38.116	41.820	1.00	2.00
ATOM	157	OG1 THR	30	59.337	36.982	42.408	1.00	2.00
ATOM	158	CG2 THR	30	57.763	38.661	42.827	1.00	2.00
ATOM	159	C THR	30	56.951	36.601	40.674	1.00	6.81
ATOM	160	O THR	30	55.774	36.924	40.814	1.00	8.70
ATOM	161	N GLU	31	57.342	35.326	40.665	1.00	7.95
ATOM	162	CA GLU	31	56.378	34.219	40.786	1.00	8.18
ATOM	163	CB GLU	31	56.577	33.240	39.650	1.00	7.89
ATOM	164	CG GLU	31	56.490	33.821	38.286	1.00	8.99
ATOM	165	CD GLU	31	56.651	32.750	37.248	1.00	10.58
ATOM	166	OE1 GLU	31	57.538	32.875	36.395	1.00	13.03
ATOM	167	OE2 GLU	31	55.916	31.753	37.302	1.00	14.01
ATOM	168	C GLU	31	56.453	32.432	42.079	1.00	8.38
ATOM	169	O GLU	31	55.437	32.940	42.582	1.00	9.78
ATOM	170	N ARG	32	57.678	33.064	42.416	1.00	7.19
ATOM	171	CA ARG	32	58.006	32.390	43.670	1.00	8.64
ATOM	172	CB ARG	32	58.844	31.154	43.405	1.00	9.16
ATOM	173	CG ARG	32	58.284	30.364	42.261	1.00	10.75
ATOM	174	CD ARG	32	58.376	28.894	42.469	1.00	11.21
ATOM	175	NE ARG	32	57.070	28.271	42.295	1.00	13.52
ATOM	176	CZ ARG	32	56.328	28.350	41.187	1.00	16.55
ATOM	177	NH1 ARG	32	56.763	29.036	40.128	1.00	17.12
ATOM	178	NH2 ARG	32	55.145	27.734	41.128	1.00	17.67
ATOM	179	C ARG	32	58.834	33.536	44.224	1.00	9.21
ATOM	180	O ARG	32	59.004	34.526	43.520	1.00	13.37
ATOM	181	N LEU	33	59.382	33.499	45.416	1.00	7.72
ATOM	182	CA LEU	33	60.084	34.736	45.716	1.00	8.01
ATOM	183	CB LEU	33	59.536	35.403	46.986	1.00	7.85
ATOM	184	CG LEU	33	58.323	36.310	46.699	1.00	2.00
ATOM	185	CD1 LEU	33	57.061	35.584	47.032	1.00	3.91
ATOM	186	CD2 LEU	33	58.381	37.604	47.464	1.00	2.00
ATOM	187	C LEU	33	61.610	34.893	45.506	1.00	8.52
ATOM	188	O LEU	33	62.269	35.702	46.168	1.00	10.67
ATOM	189	N GLU	34	62.130	34.174	44.516	1.00	6.25
ATOM	190	CA GLU	34	63.539	34.210	44.144	1.00	8.09
ATOM	191	CB GLU	34	64.315	32.005	44.723	1.00	10.89
ATOM	192	CG GLU	34	63.518	31.931	45.547	1.00	18.21
ATOM	193	CD GLU	34	62.754	30.858	44.699	1.00	21.61
ATOM	194	OE1 GLU	34	61.810	30.224	45.257	1.00	22.26
ATOM	195	OE2 GLU	34	63.082	30.645	43.494	1.00	22.29
ATOM	196	C GLU	34	63.678	34.239	42.594	1.00	7.89
ATOM	197	O GLU	34	64.413	33.459	42.016	1.00	10.91
ATOM	198	N ASP	35	62.978	35.150	41.933	1.00	6.40
ATOM	199	CA ASP	35	62.981	35.244	40.483	1.00	4.88
ATOM	200	CB ASP	35	62.215	34.034	39.895	1.00	5.00
ATOM	201	CG ASP	35	60.678	34.189	39.957	1.00	6.69
ATOM	202	OD1 ASP	35	60.055	34.542	38.912	1.00	6.86
ATOM	203	OD2 ASP	35	60.102	33.911	41.025	1.00	2.00
ATOM	204	C ASP	35	62.336	36.566	40.016	1.00	3.42
ATOM	205	O ASP	35	61.563	37.153	40.731	1.00	4.41
ATOM	206	N LEU	36	62.677	37.046	38.834	1.00	2.00
ATOM	207	CA LEU	36	62.098	38.272	38.317	1.00	2.00
ATOM	208	CB LEU	36	62.902	39.484	38.745	1.00	2.00
ATOM	209	CG LEU	36	62.219	40.825	38.490	1.00	2.40
ATOM	210	CD1 LEU	36	60.994	40.997	39.365	1.00	2.31
ATOM	211	CD2 LEU	36	63.184	41.343	38.762	1.00	2.00
ATOM	212	C LEU	36	62.119	38.170	36.803	1.00	3.03
ATOM	213	O LEU	36	63.071	37.640	36.241	1.00	3.65
ATOM	214	N VAL	37	61.036	38.589	36.151	1.00	3.46
ATOM	215	CA VAL	37	60.960	38.559	34.707	1.00	2.00
ATOM	216	CB VAL	37	59.866	37.575	34.206	1.00	2.00
ATOM	217	CG1 VAL	37	60.007	37.337	32.699	1.00	2.00
ATOM	218	CG2 VAL	37	59.957	36.271	34.942	1.00	2.00
ATOM	219	C VAL	37	60.555	39.970	34.329	1.00	3.89
ATOM	220	O VAL	37	59.738	40.553	35.043	1.00	5.63
ATOM	221	N CYS	38	61.204	40.557	33.218	1.00	2.00
ATOM	222	CA CYS	38	60.831	41.886	22.532	1.00	4.05
ATOM	223	C CYS	38	60.762	41.816	21.324	1.00	5.14
ATOM	224	O CYS	38	61.592	41.143	20.713	1.00	8.41
ATOM	225	CB CYS	38	61.808	42.975	22.213	1.00	2.98
ATOM	226	SG CYS	38	61.860	43.383	24.972	1.00	3.22

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ATOM	227	N	PHE	39	59.811	42.540	30.742	1.00	4.95	7
ATOM	228	CA	PHE	39	59.621	42.507	29.286	1.00	5.38	6
ATOM	229	CB	PHE	39	58.865	41.225	28.900	1.00	4.80	5
ATOM	230	CG	PHE	39	57.461	41.198	29.411	1.00	7.03	4
ATOM	231	CD1	PHE	39	56.416	41.686	28.636	1.00	8.61	3
ATOM	232	CD2	PHE	39	57.190	40.807	20.709	1.00	7.97	2
ATOM	233	CE1	PHE	39	55.123	41.795	29.153	1.00	9.47	1
ATOM	234	CE2	PHE	39	55.896	40.917	31.228	1.00	9.28	0
ATOM	235	CZ	PHE	39	54.868	41.411	30.451	1.00	8.72	0
ATOM	236	C	PHE	39	58.826	43.713	28.794	1.00	3.79	0
ATOM	237	O	PHE	39	58.262	44.451	29.560	1.00	4.29	0
ATOM	238	N	TRP	40	58.837	43.926	27.490	1.00	3.45	0
ATOM	239	CA	TRP	40	58.084	44.996	26.846	1.00	4.71	0
ATOM	240	CB	TRP	40	58.826	46.352	26.872	1.00	4.45	0
ATOM	241	CG	TRP	40	60.014	46.517	25.928	1.00	7.44	0
ATOM	242	CD2	TRP	40	61.386	46.185	26.200	1.00	9.31	0
ATOM	243	CE2	TRP	40	62.143	46.555	25.062	1.00	6.04	0
ATOM	244	CE3	TRP	40	62.049	45.595	27.294	1.00	10.26	0
ATOM	245	CD1	TRP	40	60.003	47.056	24.661	1.00	8.12	0
ATOM	246	NE1	TRP	40	61.277	47.087	24.144	1.00	6.99	0
ATOM	247	CZ2	TRP	40	63.527	46.358	24.989	1.00	10.83	0
ATOM	248	CZ3	TRP	40	63.431	45.395	27.217	1.00	10.61	0
ATOM	249	CH2	TRP	40	64.152	45.780	26.068	1.00	11.43	0
ATOM	250	C	TRP	40	57.785	44.539	25.418	1.00	5.55	0
ATOM	251	O	TRP	40	58.530	43.761	24.824	1.00	4.51	0
ATOM	252	N	GLU	41	56.625	44.914	24.914	1.00	7.98	0
ATOM	253	CA	GLU	41	56.267	44.533	23.556	1.00	3.54	0
ATOM	254	CB	GLU	41	54.898	42.840	23.555	1.00	7.91	0
ATOM	255	CG	GLU	41	54.860	42.586	24.450	1.00	11.77	0
ATOM	256	CD	GLU	41	53.619	41.687	24.254	1.00	13.67	0
ATOM	257	OE1	GLU	41	53.418	40.748	25.055	1.00	15.11	0
ATOM	258	OE2	GLU	41	52.843	41.891	23.301	1.00	17.90	0
ATOM	259	C	GLU	41	56.335	45.715	22.558	1.00	9.08	0
ATOM	260	O	GLU	41	56.456	46.888	22.956	1.00	8.71	0
ATOM	261	N	GLU	42	56.403	45.389	21.271	1.00	8.40	0
ATOM	262	CA	GLU	42	56.426	46.399	20.211	1.00	8.64	0
ATOM	263	CB	GLU	42	57.729	47.207	20.227	1.00	6.56	0
ATOM	264	CG	GLU	42	58.974	46.393	20.511	1.00	5.93	0
ATOM	265	CD	GLU	42	60.242	47.114	20.115	1.00	7.01	0
ATOM	266	OE1	GLU	42	61.019	46.519	19.371	1.00	9.43	0
ATOM	267	OE2	GLU	42	60.470	48.271	20.519	1.00	6.13	0
ATOM	268	C	GLU	42	56.167	45.737	18.853	1.00	9.90	0
ATOM	269	O	GLU	42	55.880	44.532	18.795	1.00	9.59	0
ATOM	270	N	ALA	43	56.243	46.514	17.771	1.00	10.98	0
ATOM	271	CA	ALA	43	55.988	46.007	16.400	1.00	12.17	0
ATOM	272	CB	ALA	43	55.513	47.145	15.515	1.00	12.56	0
ATOM	273	C	ALA	43	57.164	45.291	15.731	1.00	10.71	0
ATOM	274	O	ALA	43	58.309	45.683	15.930	1.00	13.41	0
ATOM	275	N	ALA	44	56.878	44.282	14.903	1.00	3.23	0
ATOM	276	CA	ALA	44	57.928	43.514	14.208	1.00	3.02	0
ATOM	277	CB	ALA	44	57.326	42.507	13.263	1.00	4.97	0
ATOM	278	C	ALA	44	58.828	44.442	13.438	1.00	8.51	0
ATOM	279	O	ALA	44	58.407	45.534	13.047	1.00	9.27	0
ATOM	280	N	SER	45	60.086	44.068	13.275	1.00	9.06	0
ATOM	281	CA	SER	45	60.962	44.926	12.508	1.00	10.80	0
ATOM	282	CB	SER	45	61.618	46.002	13.354	1.00	11.24	0
ATOM	283	OG	SER	45	61.479	47.244	12.695	1.00	10.08	0
ATOM	284	C	SER	45	61.996	44.207	11.683	1.00	13.63	0
ATOM	285	O	SER	45	62.599	43.221	12.124	1.00	15.72	0
ATOM	286	N	ALA	46	62.112	44.671	10.435	1.00	14.88	0
ATOM	287	CA	ALA	46	63.041	44.134	9.469	1.00	14.41	0
ATOM	288	CB	ALA	46	62.810	44.781	8.127	1.00	17.01	0
ATOM	289	C	ALA	46	64.379	44.538	10.028	1.00	15.43	0
ATOM	290	O	ALA	46	64.657	45.746	10.203	1.00	16.87	0
ATOM	291	N	GLY	47	65.140	43.525	10.433	1.00	11.71	0
ATOM	292	CA	GLY	47	66.450	43.762	11.009	1.00	15.77	0
ATOM	293	C	GLY	47	66.558	44.415	12.400	1.00	15.13	0
ATOM	294	O	GLY	47	67.221	45.457	12.546	1.00	16.83	0
ATOM	295	N	VAL	48	65.872	43.843	13.399	1.00	13.97	0
ATOM	296	CA	VAL	48	65.950	44.302	14.799	1.00	17.23	0
ATOM	297	CB	VAL	48	64.825	45.230	15.231	1.00	8.24	0
ATOM	298	CG1	VAL	48	64.572	45.071	16.701	1.00	8.08	0
ATOM	299	CG2	VAL	48	65.216	46.550	14.964	1.00	6.13	0
ATOM	300	C	VAL	48	65.904	43.060	15.642	1.00	3.63	0
ATOM	301	O	VAL	48	65.062	42.183	15.443	1.00	3.93	0
ATOM	302	N	GLY	49	66.882	42.949	16.521	1.00	3.43	0
ATOM	303	CA	GLY	49	66.948	41.798	17.393	1.00	7.27	0
ATOM	304	C	GLY	49	67.199	42.211	18.829	1.00	5.14	0



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ATOM	305	O	GLY	49	67.294	43.396	19.152	1.00	3.06	5
ATOM	306	N	PRO	50	67.274	41.234	19.732	1.00	4.49	7
ATOM	307	CD	PRO	50	67.104	39.790	19.536	1.00	2.00	5
ATOM	308	CA	PRO	50	67.519	41.540	21.125	1.00	2.99	5
ATOM	309	CB	PRO	50	67.545	40.158	21.762	1.00	3.97	5
ATOM	310	CG	PRO	50	67.935	39.264	20.632	1.00	2.00	5
ATOM	311	C	PRO	50	68.837	42.307	21.315	1.00	4.87	5
ATOM	312	O	PRO	50	68.962	43.122	22.217	1.00	7.36	5
ATOM	313	N	GLY	51	69.787	42.100	20.403	1.00	5.60	7
ATOM	314	CA	GLY	51	71.059	42.792	20.477	1.00	2.83	5
ATOM	315	C	GLY	51	70.991	44.263	20.103	1.00	3.36	5
ATOM	316	O	GLY	51	72.025	44.910	19.956	1.00	5.85	5
ATOM	317	N	ASN	52	69.792	44.815	19.968	1.00	2.00	7
ATOM	318	CA	ASN	52	69.670	46.211	19.604	1.00	2.00	5
ATOM	319	CB	ASN	52	68.527	46.401	18.633	1.00	3.33	5
ATOM	320	CG	ASN	52	68.768	47.534	17.666	1.00	7.97	5
ATOM	321	OD1	ASN	52	69.233	47.311	16.538	1.00	12.55	5
ATOM	322	ND2	ASN	52	68.442	48.753	18.079	1.00	10.05	7
ATOM	323	C	ASN	52	69.505	47.144	20.797	1.00	3.59	5
ATOM	324	O	ASN	52	69.524	48.359	20.638	1.00	2.00	5
ATOM	325	N	TYR	53	69.286	46.573	21.985	1.00	5.70	7
ATOM	326	CA	TYR	53	69.146	47.350	23.229	1.00	5.58	5
ATOM	327	CB	TYR	53	67.707	47.412	23.770	1.00	5.70	5
ATOM	328	CG	TYR	53	66.615	47.547	22.768	1.00	4.84	5
ATOM	329	CD1	TYR	53	66.067	46.414	22.188	1.00	6.02	5
ATOM	330	CE1	TYR	53	65.080	46.495	21.282	1.00	5.48	5
ATOM	331	CD2	TYR	53	66.123	48.789	22.405	1.00	5.30	5
ATOM	332	CE2	TYR	53	65.118	48.891	21.495	1.00	6.56	5
ATOM	333	C2	TYR	53	64.598	47.729	20.929	1.00	8.17	5
ATOM	334	OH	TYR	53	63.590	47.767	19.987	1.00	12.54	5
ATOM	335	C	TYR	53	69.943	46.667	24.308	1.00	3.83	5
ATOM	336	O	TYR	53	70.176	45.465	24.245	1.00	4.09	5
ATOM	337	N	SER	54	70.257	47.428	25.346	1.00	3.81	7
ATOM	338	CA	SER	54	70.977	46.921	26.501	1.00	6.59	5
ATOM	339	CB	SER	54	72.296	47.682	26.710	1.00	8.72	5
ATOM	340	OG	SER	54	73.405	46.867	26.341	1.00	13.32	5
ATOM	341	C	SER	54	70.077	47.035	27.726	1.00	4.52	5
ATOM	342	O	SER	54	69.495	48.089	27.982	1.00	5.58	5
ATOM	343	N	PHE	55	69.931	45.926	28.443	1.00	3.52	7
ATOM	344	CA	PHE	55	69.095	45.878	29.641	1.00	3.38	5
ATOM	345	CB	PHE	55	68.141	44.676	29.574	1.00	6.11	5
ATOM	346	CG	PHE	55	67.052	44.700	30.596	1.00	6.96	5
ATOM	347	CD1	PHE	55	65.741	44.865	30.214	1.00	10.17	5
ATOM	348	CD2	PHE	55	67.330	44.547	31.929	1.00	8.73	5
ATOM	349	CE1	PHE	55	64.713	44.879	31.154	1.00	12.64	5
ATOM	350	CE2	PHE	55	66.317	44.561	32.874	1.00	8.02	5
ATOM	351	C2	PHE	55	65.007	44.728	32.490	1.00	8.93	5
ATOM	352	C	PHE	55	69.942	45.779	30.891	1.00	2.90	5
ATOM	353	O	PHE	55	70.476	44.710	31.200	1.00	2.00	5
ATOM	354	N	SER	56	70.083	46.892	31.595	1.00	2.00	7
ATOM	355	CA	SER	56	70.854	46.862	32.818	1.00	5.40	5
ATOM	356	CB	SER	56	72.159	47.651	32.681	1.00	6.39	5
ATOM	357	OG	SER	56	71.950	48.939	32.162	1.00	9.05	5
ATOM	358	C	SER	56	70.089	47.214	34.108	1.00	8.43	5
ATOM	359	O	SER	56	69.080	47.943	34.098	1.00	7.21	5
ATOM	360	N	TYR	57	70.546	46.635	35.213	1.00	7.52	7
ATOM	361	CA	TYR	57	69.915	46.856	36.495	1.00	8.61	5
ATOM	362	CB	TYR	57	69.091	45.621	36.883	1.00	3.65	5
ATOM	363	CG	TYR	57	69.863	44.334	37.004	1.00	4.17	5
ATOM	364	CD1	TYR	57	70.254	43.835	38.254	1.00	2.00	5
ATOM	365	CE1	TYR	57	70.865	42.587	38.384	1.00	2.00	5
ATOM	366	CD2	TYR	57	70.115	43.560	35.894	1.00	4.11	5
ATOM	367	CE2	TYR	57	70.729	42.316	36.020	1.00	2.48	5
ATOM	368	C2	TYR	57	71.096	41.834	37.260	1.00	2.00	5
ATOM	369	OH	TYR	57	71.673	40.591	37.334	1.00	2.00	5
ATOM	370	C	TYR	57	70.885	47.253	37.616	1.00	10.04	5
ATOM	371	O	TYR	57	72.092	47.181	37.466	1.00	11.97	5
ATOM	372	N	GLN	58	70.353	47.781	38.705	1.00	11.03	5
ATOM	373	CA	GLN	58	71.181	48.143	39.832	1.00	9.11	5
ATOM	374	CB	GLN	58	71.613	49.592	39.754	1.00	10.64	5
ATOM	375	CG	GLN	58	72.167	50.091	41.062	1.00	13.28	5
ATOM	376	CD	GLN	58	72.827	51.436	40.954	1.00	13.57	5
ATOM	377	OE1	GLN	58	72.165	52.472	40.844	1.00	15.62	5
ATOM	378	NE2	GLN	58	74.147	51.435	41.026	1.00	14.36	5
ATOM	379	C	GLN	58	70.430	47.886	41.123	1.00	8.05	5
ATOM	380	O	GLN	58	69.489	48.583	41.468	1.00	7.60	5
ATOM	381	N	LEU	59	70.777	46.798	41.769	1.00	8.41	5
ATOM	382	CA	LEU	59	70.183	46.435	43.036	1.00	6.43	5

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ATOM	383	CB LEU	59	70.534	44.993	43.313	1.00	4.10
ATOM	384	CG LEU	59	69.811	44.344	44.446	1.00	2.46
ATOM	385	CD1 LEU	59	68.343	44.461	44.227	1.00	3.98
ATOM	386	CD2 LEU	59	70.246	42.909	44.462	1.00	6.03
ATOM	387	C LEU	59	70.926	47.335	43.995	1.00	9.36
ATOM	388	O LEU	59	72.125	47.210	44.085	1.00	9.93
ATOM	389	N GLU	60	70.227	48.253	44.667	1.00	11.94
ATOM	390	CA GLU	60	70.844	49.221	45.603	1.00	13.27
ATOM	391	CB GLU	60	69.852	49.697	46.643	1.00	14.05
ATOM	392	CG GLU	60	70.448	50.769	47.531	1.00	15.91
ATOM	393	CD GLU	60	69.443	51.351	48.510	1.00	16.83
ATOM	394	OE1 GLU	60	69.263	50.755	49.607	1.00	16.52
ATOM	395	OE2 GLU	60	68.852	52.410	48.181	1.00	15.77
ATOM	396	C GLU	60	72.159	48.859	46.315	1.00	14.73
ATOM	397	O GLU	60	72.200	47.971	47.189	1.00	14.00
ATOM	398	N ASP	61	73.193	49.638	45.973	1.00	16.22
ATOM	399	CA ASP	61	74.569	49.501	46.452	1.00	17.32
ATOM	400	CB ASP	61	74.624	49.151	47.930	1.00	22.61
ATOM	401	CG ASP	61	74.287	50.345	48.814	1.00	26.60
ATOM	402	OD1 ASP	61	74.262	50.144	50.054	1.00	30.15
ATOM	403	OD2 ASP	61	74.036	51.470	48.271	1.00	27.62
ATOM	404	C ASP	61	75.390	48.539	45.610	1.00	16.14
ATOM	405	O ASP	61	76.382	48.742	45.423	1.00	16.58
ATOM	406	N GLU	62	74.758	47.476	45.130	1.00	14.78
ATOM	407	CA GLU	62	75.402	46.524	44.223	1.00	13.68
ATOM	408	CB GLU	62	74.418	45.359	43.931	1.00	15.90
ATOM	409	CG GLU	62	74.592	44.612	42.585	1.00	20.15
ATOM	410	CD GLU	62	73.574	44.998	41.452	1.00	18.81
ATOM	411	OE1 GLU	62	73.324	46.202	41.202	1.00	19.09
ATOM	412	OE2 GLU	62	73.047	44.078	40.788	1.00	17.28
ATOM	413	C GLU	62	75.709	47.363	42.947	1.00	10.99
ATOM	414	O GLU	62	75.069	48.402	42.704	1.00	11.23
ATOM	415	N PRO	63	76.744	46.984	42.173	1.00	9.01
ATOM	416	CD PRO	63	77.785	45.973	42.435	1.00	9.66
ATOM	417	CA PRO	63	77.069	47.740	40.959	1.00	8.47
ATOM	418	CB PRO	63	78.517	47.322	40.691	1.00	5.33
ATOM	419	CG PRO	63	78.504	45.895	41.103	1.00	7.09
ATOM	420	C PRO	63	76.146	47.407	39.779	1.00	6.19
ATOM	421	O PRO	63	75.473	46.366	39.775	1.00	4.91
ATOM	422	N TRP	64	76.119	48.300	38.788	1.00	3.37
ATOM	423	CA TRP	64	75.298	48.092	37.613	1.00	2.00
ATOM	424	CB TRP	64	75.441	49.259	36.645	1.00	2.40
ATOM	425	CG TRP	64	74.591	50.490	36.923	1.00	2.00
ATOM	426	CD2 TRP	64	73.181	50.651	36.678	1.00	2.00
ATOM	427	CE2 TRP	64	72.845	51.972	37.050	1.00	2.28
ATOM	428	CE3 TRP	64	72.174	49.811	36.186	1.00	2.18
ATOM	429	CD1 TRP	64	75.027	51.682	37.410	1.00	2.00
ATOM	430	NE1 TRP	64	72.995	52.573	37.487	1.00	2.00
ATOM	431	CZ2 TRP	64	71.537	52.476	36.950	1.00	2.00
ATOM	432	CZ3 TRP	64	70.878	50.314	36.087	1.00	2.49
ATOM	433	CH2 TRP	64	70.575	51.636	36.471	1.00	2.00
ATOM	434	C TRP	64	75.706	46.815	36.903	1.00	2.00
ATOM	435	O TRP	64	76.877	46.528	36.736	1.00	2.00
ATOM	436	N LYS	65	74.704	46.036	36.524	1.00	2.00
ATOM	437	CA LYS	65	74.909	44.793	35.803	1.00	2.00
ATOM	438	CB LYS	65	74.603	43.597	36.668	1.00	2.61
ATOM	439	CG LYS	65	75.611	43.306	37.673	1.00	3.35
ATOM	440	CD LYS	65	75.207	42.082	38.401	1.00	4.33
ATOM	441	CE LYS	65	76.204	41.795	39.488	1.00	10.13
ATOM	442	NZ LYS	65	76.452	43.031	40.293	1.00	15.09
ATOM	443	C LYS	65	74.017	44.725	34.584	1.00	2.00
ATOM	444	O LYS	65	73.125	45.534	34.416	1.00	2.81
ATOM	445	N LEU	66	74.201	43.692	33.780	1.00	2.51
ATOM	446	CA LEU	66	72.421	43.532	32.558	1.00	3.38
ATOM	447	CB LEU	66	74.342	43.586	31.340	1.00	2.07
ATOM	448	CG LEU	66	75.135	44.851	31.138	1.00	2.42
ATOM	449	CD1 LEU	66	76.363	44.485	30.416	1.00	5.47
ATOM	450	CD2 LEU	66	74.227	45.880	30.383	1.00	2.99
ATOM	451	C LEU	66	72.651	42.234	32.492	1.00	3.16
ATOM	452	O LEU	66	73.125	41.193	32.943	1.00	2.56
ATOM	453	N CYS	67	71.479	42.283	31.885	1.00	4.64
ATOM	454	CA CYS	67	70.686	41.090	31.708	1.00	8.30
ATOM	455	C CYS	67	70.569	40.952	30.191	1.00	9.34
ATOM	456	O CYS	67	70.506	41.960	29.512	1.00	11.12
ATOM	457	CB CYS	67	69.331	41.270	32.363	1.00	9.68
ATOM	458	SG CYS	67	68.297	39.785	32.300	1.00	9.98
ATOM	459	N ARG	68	70.672	39.729	29.649	1.00	10.88
ATOM	460	CA ARG	68	70.567	39.524	28.187	1.00	11.77

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ATOM	461	CB	ARG	68	71.380	38.359	27.627	1.00	15.15		
ATOM	462	CG	ARG	68	71.366	38.376	26.053	1.00	20.38		
ATOM	463	CD	ARG	68	71.858	37.102	25.359	1.00	21.17		
ATOM	464	NE	ARG	68	71.010	35.943	25.653	1.00	25.20		
ATOM	465	CZ	ARG	68	71.437	34.837	26.288	1.00	27.66		
ATOM	466	NH1	ARG	68	72.710	34.732	26.705	1.00	28.62		
ATOM	467	NH2	ARG	68	70.601	33.818	26.498	1.00	27.68		
ATOM	468	C	ARG	68	69.143	39.327	27.751	1.00	9.76		
ATOM	469	O	ARG	68	68.449	38.504	28.317	1.00	9.75		
ATOM	470	N	LEU	69	68.762	40.027	26.684	1.00	8.16		
ATOM	471	CA	LEU	69	67.428	39.983	26.121	1.00	5.24		
ATOM	472	CB	LEU	69	67.137	41.247	25.328	1.00	4.64		
ATOM	473	CG	LEU	69	67.431	42.587	25.980	1.00	5.82		
ATOM	474	CD1	LEU	69	67.302	43.727	25.026	1.00	9.48		
ATOM	475	CD2	LEU	69	66.498	42.773	27.111	1.00	9.06		
ATOM	476	C	LEU	69	67.222	38.794	25.221	1.00	6.45		
ATOM	477	O	LEU	69	68.175	38.217	24.655	1.00	6.60		
ATOM	478	N	HIS	70	65.947	38.430	25.133	1.00	6.17		
ATOM	479	CA	HIS	70	65.448	37.374	24.296	1.00	4.34		
ATOM	480	CB	HIS	70	64.792	36.308	25.103	1.00	3.32		
ATOM	481	CG	HIS	70	65.759	35.494	25.871	1.00	4.94		
ATOM	482	CD2	HIS	70	66.779	34.706	25.460	1.00	7.46		
ATOM	483	ND1	HIS	70	65.759	35.444	27.243	1.00	8.83		
ATOM	484	CE1	HIS	70	66.738	34.653	27.650	1.00	9.22		
ATOM	485	NE2	HIS	70	67.372	34.193	26.586	1.00	6.78		
ATOM	486	C	HIS	70	64.407	38.097	23.546	1.00	6.62		
ATOM	487	O	HIS	70	64.129	39.240	23.863	1.00	7.62		
ATOM	488	N	GLN	71	63.871	37.453	22.520	1.00	10.06		
ATOM	489	CA	GLN	71	62.828	36.038	21.676	1.00	12.44		
ATOM	490	CB	GLN	71	63.449	38.691	20.442	1.00	12.64		
ATOM	491	CG	GLN	71	62.523	39.628	19.675	1.00	12.33		
ATOM	492	CD	GLN	71	63.193	40.157	18.423	1.00	11.98		
ATOM	493	OE1	GLN	71	63.256	41.364	18.185	1.00	14.18		
ATOM	494	NE2	GLN	71	63.741	39.254	17.638	1.00	13.04		
ATOM	495	C	GLN	71	61.867	36.915	21.278	1.00	14.54		
ATOM	496	O	GLN	71	62.293	35.846	20.828	1.00	13.15		
ATOM	497	N	ALA	72	60.576	37.148	21.510	1.00	16.60		
ATOM	498	CA	ALA	72	59.540	36.163	21.222	1.00	17.29		
ATOM	499	CB	ALA	72	59.106	35.462	22.513	1.00	18.25		
ATOM	500	C	ALA	72	58.339	36.816	20.552	1.00	17.09		
ATOM	501	O	ALA	72	57.962	37.949	20.890	1.00	17.99		
ATOM	502	N	PRO	73	57.770	36.140	19.535	1.00	15.70		
ATOM	503	CD	PRO	73	58.266	34.944	18.833	1.00	15.56		
ATOM	504	CA	PRO	73	56.618	36.681	18.835	1.00	14.26		
ATOM	505	CB	PRO	73	56.539	35.789	17.608	1.00	14.62		
ATOM	506	CG	PRO	73	57.057	34.500	18.096	1.00	14.52		
ATOM	507	C	PRO	73	55.292	36.586	19.707	1.00	13.69		
ATOM	508	O	PRO	73	55.295	35.678	20.522	1.00	16.10		
ATOM	509	N	THR	74	54.568	37.632	19.628	1.00	12.65		
ATOM	510	CA	THR	74	53.304	37.789	20.338	1.00	11.59		
ATOM	511	CB	THR	74	52.987	39.276	20.518	1.00	8.94		
ATOM	512	CG1	THR	74	54.100	39.935	21.092	1.00	12.22		
ATOM	513	CG2	THR	74	51.790	39.484	21.423	1.00	13.10		
ATOM	514	C	THR	74	52.216	37.289	19.382	1.00	13.56		
ATOM	515	O	THR	74	52.234	37.637	18.198	1.00	16.99		
ATOM	516	N	ALA	75	51.237	36.542	19.885	1.00	12.64		
ATOM	517	CA	ALA	75	50.131	36.076	19.045	1.00	10.05		
ATOM	518	CB	ALA	75	48.995	35.578	19.905	1.00	10.80		
ATOM	519	C	ALA	75	49.612	37.152	18.102	1.00	8.70		
ATOM	520	O	ALA	75	49.256	36.837	16.987	1.00	12.33		
ATOM	521	N	ARG	76	49.583	38.410	18.545	1.00	9.12		
ATOM	522	CA	ARG	76	49.107	39.552	17.744	1.00	10.37		
ATOM	523	CB	ARG	76	48.870	40.786	18.606	1.00	10.98		
ATOM	524	CG	ARG	76	47.709	40.722	19.529	1.00	16.38		
ATOM	525	CD	ARG	76	47.936	41.676	20.736	1.00	21.72		
ATOM	526	NE	ARG	76	47.298	41.163	21.957	1.00	23.03		
ATOM	527	CZ	ARG	76	47.700	40.066	22.605	1.00	25.34		
ATOM	528	NH1	ARG	76	48.745	39.355	22.160	1.00	25.68		
ATOM	529	NH2	ARG	76	47.065	39.679	23.712	1.00	28.25		
ATOM	530	C	ARG	76	50.026	40.042	16.641	1.00	12.35		
ATOM	531	O	ARG	76	49.680	41.002	15.961	1.00	15.69		
ATOM	532	N	GLY	77	51.223	39.489	16.508	1.00	12.77		
ATOM	533	CA	GLY	77	52.121	39.982	15.473	1.00	11.39		
ATOM	534	C	GLY	77	53.079	41.083	15.909	1.00	11.38		
ATOM	535	O	GLY	77	53.633	41.814	15.102	1.00	10.58		
ATOM	536	N	ALA	78	53.242	41.226	17.208	1.00	12.04		
ATOM	537	CA	ALA	78	54.158	42.210	17.759	1.00	11.50		
ATOM	538	CB	ALA	78	53.465	43.041	18.831	1.00	10.28		

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ATOM	539	C ALA	78	55.263	41.329	18.357	1.00	11.11 6
ATOM	540	O ALA	78	55.080	40.106	18.495	1.00	10.01 6
ATOM	541	N VAL	79	56.418	41.923	18.640	1.00	9.69 7
ATOM	542	CA VAL	79	57.546	41.178	19.192	1.00	7.22 6
ATOM	543	CB VAL	79	58.844	41.391	18.354	1.00	6.05 6
ATOM	544	CG1 VAL	79	58.706	40.741	17.024	1.00	6.29 6
ATOM	545	CG2 VAL	79	59.135	42.848	18.171	1.00	5.80 6
ATOM	546	C VAL	79	57.786	41.500	20.672	1.00	5.75 6
ATOM	547	O VAL	79	57.633	42.637	21.125	1.00	4.75 6
ATOM	548	N ARG	80	58.207	40.491	21.403	1.00	4.34 7
ATOM	549	CA ARG	80	58.420	40.648	22.813	1.00	7.09 6
ATOM	550	CB ARG	80	57.507	39.672	23.550	1.00	8.65 6
ATOM	551	CG ARG	80	57.465	39.838	25.052	1.00	7.34 6
ATOM	552	CD ARG	80	56.674	38.710	25.630	1.00	6.89 6
ATOM	553	NE ARG	80	55.272	38.809	25.237	1.00	6.67 7
ATOM	554	CZ ARG	80	54.415	37.809	25.313	1.00	4.11 6
ATOM	555	NH1 ARG	80	54.829	36.631	25.743	1.00	5.04 7
ATOM	556	NH2 ARG	80	53.142	38.017	25.063	1.00	2.00 7
ATOM	557	C ARG	80	59.846	40.484	23.297	1.00	5.10 6
ATOM	558	O ARG	80	60.466	39.434	23.114	1.00	3.87 9
ATOM	559	N PHE	81	60.346	41.519	23.951	1.00	4.32 7
ATOM	560	CA PHE	81	61.688	41.481	24.488	1.00	5.56 6
ATOM	561	CB PHE	81	62.385	42.814	24.305	1.00	4.97 6
ATOM	562	CG PHE	81	62.744	43.102	22.915	1.00	5.07 6
ATOM	563	CD1 PHE	81	61.861	43.781	22.091	1.00	6.98 6
ATOM	564	CD2 PHE	81	63.947	42.670	22.409	1.00	7.17 6
ATOM	565	CE1 PHE	81	62.164	44.030	20.763	1.00	7.52 6
ATOM	566	CE2 PHE	81	64.275	42.908	21.086	1.00	10.89 6
ATOM	567	CZ PHE	81	63.374	43.594	20.251	1.00	10.08 6
ATOM	568	C PHE	81	61.546	41.209	25.955	1.00	7.23 6
ATOM	569	O PHE	81	60.725	41.848	26.604	1.00	8.68 8
ATOM	570	N TRP	82	62.301	40.240	26.469	1.00	7.82 7
ATOM	571	CA TRP	82	62.263	39.911	27.891	1.00	8.83 6
ATOM	572	CB TRP	82	61.252	38.789	28.199	1.00	9.85 6
ATOM	573	CG TRP	82	61.585	37.412	27.697	1.00	12.09 6
ATOM	574	CD2 TRP	82	62.234	36.372	28.428	1.00	11.52 6
ATOM	575	CE2 TRP	82	62.328	35.248	27.577	1.00	13.27 6
ATOM	576	CE3 TRP	82	62.744	36.277	29.722	1.00	15.01 6
ATOM	577	CD1 TRP	82	61.304	36.888	26.453	1.00	14.64 6
ATOM	578	NE1 TRP	82	61.750	35.581	26.378	1.00	12.57 7
ATOM	579	CZ2 TRP	82	62.919	34.048	27.987	1.00	17.05 6
ATOM	580	CZ3 TRP	82	63.333	35.071	30.137	1.00	16.75 6
ATOM	581	CH2 TRP	82	63.415	33.980	29.272	1.00	17.82 6
ATOM	582	C TRP	82	63.656	39.561	28.371	1.00	8.65 6
ATOM	583	O TRP	82	64.606	39.733	27.623	1.00	7.22 6
ATOM	584	N CYS	83	63.769	39.156	29.635	1.00	7.16 7
ATOM	585	CA CYS	83	65.024	38.749	30.282	1.00	6.52 6
ATOM	586	C CYS	83	64.632	38.373	31.702	1.00	4.93 6
ATOM	587	O CYS	83	63.737	38.969	32.271	1.00	5.96 6
ATOM	588	CB CYS	83	66.026	39.909	30.319	1.00	7.79 6
ATOM	589	SG CYS	83	66.435	40.538	31.992	1.00	15.35 16
ATOM	590	N SER	84	65.241	37.353	32.258	1.00	3.11 7
ATOM	591	CA SER	84	64.904	36.980	33.610	1.00	4.32 6
ATOM	592	CB SER	84	64.396	35.555	33.658	1.00	5.70 6
ATOM	593	OG SER	84	65.095	34.752	32.731	1.00	12.40 6
ATOM	594	C SER	84	66.124	37.135	34.483	1.00	7.36 6
ATOM	595	O SER	84	67.172	36.544	34.190	1.00	11.62 6
ATOM	596	N LEU	85	66.002	37.940	35.546	1.00	7.67 7
ATOM	597	CA LEU	85	67.115	38.209	36.457	1.00	4.88 6
ATOM	598	CB LEU	85	66.677	39.160	37.546	1.00	3.56 6
ATOM	599	CG LEU	85	66.732	40.624	37.197	1.00	5.43 6
ATOM	600	CD1 LEU	85	67.012	41.388	38.482	1.00	7.87 6
ATOM	601	CD2 LEU	85	67.840	40.844	36.232	1.00	6.46 6
ATOM	602	C LEU	85	67.709	36.991	37.110	1.00	6.00 6
ATOM	603	O LEU	85	67.002	36.021	37.352	1.00	9.20 6
ATOM	604	N PRO	86	69.027	37.017	37.388	1.00	5.88 7
ATOM	605	CD PRO	86	69.953	38.092	35.989	1.00	6.07 6
ATOM	606	CA PRO	86	69.760	35.918	38.036	1.00	4.84 6
ATOM	607	CB PRO	86	71.212	36.361	37.921	1.00	3.16 6
ATOM	608	CG PRO	86	71.201	37.343	36.772	1.00	5.18 6
ATOM	609	C PRO	86	69.333	35.832	39.515	1.00	3.99 6
ATOM	610	O PRO	86	69.142	36.847	40.187	1.00	4.26 6
ATOM	611	N THR	87	69.227	34.622	40.029	1.00	4.59 7
ATOM	612	CA THR	87	68.792	34.399	41.394	1.00	6.71 6
ATOM	613	CB THR	87	68.963	32.949	41.727	1.00	8.22 6
ATOM	614	OG1 THR	87	68.497	32.183	40.607	1.00	9.20 6
ATOM	615	CG2 THR	87	68.149	32.599	42.975	1.00	11.56 6
ATOM	616	C THR	87	69.352	35.263	42.531	1.00	7.78 6

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ATOM	617	O	THR	87	68.606	35.730	43.384	1.00	9.13		
ATOM	618	N	ALA	88	70.661	35.474	42.541	1.00	8.99		
ATOM	619	CA	ALA	88	71.313	36.286	43.568	1.00	8.39		
ATOM	620	CB	ALA	88	72.812	36.176	43.419	1.00	9.06		
ATOM	621	C	ALA	88	70.922	37.752	43.497	1.00	8.97		
ATOM	622	O	ALA	88	71.441	38.573	44.247	1.00	10.83		
ATOM	623	N	ASP	89	70.030	38.090	42.578	1.00	8.36		
ATOM	624	CA	ASP	89	69.633	39.470	42.397	1.00	8.96		
ATOM	625	CB	ASP	89	70.047	39.911	40.992	1.00	7.68		
ATOM	626	CG	ASP	89	71.563	39.915	40.788	1.00	6.73		
ATOM	627	OD1	ASP	89	72.319	40.224	41.720	1.00	3.92		
ATOM	628	OD2	ASP	89	72.012	39.646	39.667	1.00	6.25		
ATOM	629	C	ASP	89	68.141	39.746	42.654	1.00	9.65		
ATOM	630	O	ASP	89	67.668	40.880	42.522	1.00	9.22		
ATOM	631	N	THR	90	67.420	38.724	43.094	1.00	7.69		
ATOM	632	CA	THR	90	66.010	38.866	43.359	1.00	5.03		
ATOM	633	CB	THR	90	65.298	37.603	42.898	1.00	3.78		
ATOM	634	OG1	THR	90	65.905	36.466	43.495	1.00	2.00		
ATOM	635	CG2	THR	90	65.464	37.445	41.430	1.00	3.18		
ATOM	636	C	THR	90	65.667	39.219	44.823	1.00	8.87		
ATOM	637	O	THR	90	64.634	38.790	45.335	1.00	11.62		
ATOM	638	N	SER	91	66.492	40.043	45.479	1.00	7.49		
ATOM	639	CA	SER	91	66.264	40.434	46.877	1.00	7.21		
ATOM	640	CB	SER	91	67.470	41.178	47.448	1.00	9.23		
ATOM	641	OG	SER	91	68.619	40.343	47.478	1.00	9.38		
ATOM	642	C	SER	91	65.008	41.265	47.033	1.00	8.55		
ATOM	643	O	SER	91	64.779	42.197	46.263	1.00	9.93		
ATOM	644	N	SER	92	64.287	41.029	48.125	1.00	8.52		
ATOM	645	CA	SER	92	63.000	41.671	48.338	1.00	6.55		
ATOM	646	CB	SER	92	62.022	40.702	49.003	1.00	7.73		
ATOM	647	OG	SER	92	61.127	40.120	48.085	1.00	9.02		
ATOM	648	C	SER	92	62.732	42.992	48.963	1.00	6.08		
ATOM	649	O	SER	92	61.652	43.499	48.744	1.00	10.02		
ATOM	650	N	PHE	93	63.600	43.581	49.764	1.00	5.40		
ATOM	651	CA	PHE	93	63.132	44.847	50.366	1.00	3.55		
ATOM	652	CB	PHE	93	62.881	44.663	51.879	1.00	2.38		
ATOM	653	CG	PHE	93	61.836	43.585	52.207	1.00	2.00		
ATOM	654	CD1	PHE	93	62.214	42.264	52.444	1.00	2.00		
ATOM	655	CD2	PHE	93	60.475	43.884	52.232	1.00	2.00		
ATOM	656	CE1	PHE	93	61.260	41.265	52.689	1.00	2.00		
ATOM	657	CE2	PHE	93	59.520	42.881	52.478	1.00	2.00		
ATOM	658	CZ	PHE	93	59.922	41.573	52.704	1.00	2.00		
ATOM	659	C	PHE	93	63.923	46.107	50.035	1.00	5.65		
ATOM	660	O	PHE	93	63.753	47.156	50.657	1.00	5.77		
ATOM	661	N	VAL	94	64.671	46.008	48.938	1.00	5.76		
ATOM	662	CA	VAL	94	65.542	47.054	48.410	1.00	4.07		
ATOM	663	CB	VAL	94	66.969	46.501	49.238	1.00	3.20		
ATOM	664	CG1	VAL	94	67.600	46.310	49.571	1.00	6.35		
ATOM	665	CG2	VAL	94	66.935	45.177	47.522	1.00	2.00		
ATOM	666	C	VAL	94	65.042	47.525	47.040	1.00	6.50		
ATOM	667	O	VAL	94	64.317	46.793	46.368	1.00	6.26		
ATOM	668	N	PRO	95	65.364	48.780	46.648	1.00	4.63		
ATOM	669	CD	PRO	95	65.947	49.823	47.507	1.00	5.07		
ATOM	670	CA	PRO	95	64.960	49.357	49.365	1.00	2.90		
ATOM	671	CB	PRO	95	65.316	50.826	45.530	1.00	2.93		
ATOM	672	CG	PRO	95	65.261	51.036	47.004	1.00	4.40		
ATOM	673	C	PRO	95	65.783	48.756	44.248	1.00	5.07		
ATOM	674	O	PRO	95	66.985	48.592	44.399	1.00	7.49		
ATOM	675	N	LEU	96	65.128	48.419	43.141	1.00	6.65		
ATOM	676	CA	LEU	96	65.776	47.852	41.957	1.00	5.19		
ATOM	677	CB	LEU	96	65.088	46.531	41.543	1.00	3.04		
ATOM	678	CG	LEU	96	65.571	45.607	40.411	1.00	2.00		
ATOM	679	CD1	LEU	96	66.945	45.060	40.642	1.00	2.00		
ATOM	680	CD2	LEU	96	64.648	44.446	40.315	1.00	2.00		
ATOM	681	C	LEU	96	65.713	48.886	40.816	1.00	5.21		
ATOM	682	O	LEU	96	64.639	49.309	40.367	1.00	5.02		
ATOM	683	N	GLU	97	66.881	49.355	40.416	1.00	8.18		
ATOM	684	CA	GLU	97	67.000	50.324	39.326	1.00	3.49		
ATOM	685	CB	GLU	97	68.315	51.069	39.476	1.00	10.17		
ATOM	686	CG	GLU	97	68.162	52.499	33.849	1.00	10.56		
ATOM	687	CD	GLU	97	67.806	53.335	33.676	1.00	12.04		
ATOM	688	OE1	GLU	97	68.087	54.545	33.734	1.00	14.20		
ATOM	689	OE2	GLU	97	67.252	52.787	37.691	1.00	17.02		
ATOM	690	C	GLU	97	66.959	49.610	37.987	1.00	8.71		
ATOM	691	O	GLU	97	67.735	48.689	37.741	1.00	9.31		
ATOM	692	N	LEU	98	66.083	50.053	37.101	1.00	3.76		
ATOM	693	CA	LEU	98	65.954	49.400	35.821	1.00	3.77		
ATOM	694	CB	LEU	98	64.592	48.695	35.754	1.00	3.21		

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ATOM	695	CG LEU	98	64.366	47.487	35.686	1.00	9.97
ATOM	696	CD1 LEU	98	62.912	47.080	35.721	1.00	9.15
ATOM	697	CD2 LEU	98	65.203	46.309	35.266	1.00	8.89
ATOM	698	C LEU	98	66.141	50.388	34.676	1.00	9.74
ATOM	699	O LEU	98	65.751	51.556	34.781	1.00	11.17
ATOM	700	N ARG	99	66.814	49.945	33.621	1.00	7.82
ATOM	701	CA ARG	99	67.050	50.799	32.467	1.00	8.42
ATOM	702	CB ARG	99	68.265	51.701	32.680	1.00	9.99
ATOM	703	CG ARG	99	68.319	52.571	33.915	1.00	13.57
ATOM	704	CD ARG	99	69.548	53.483	33.832	1.00	15.63
ATOM	705	NE ARG	99	70.798	52.717	33.766	1.00	21.42
ATOM	706	CZ ARG	99	71.623	52.634	32.709	1.00	23.75
ATOM	707	NH1 ARG	99	71.364	53.271	31.557	1.00	25.09
ATOM	708	NH2 ARG	99	72.747	51.921	32.818	1.00	24.11
ATOM	709	C ARG	99	67.294	50.002	31.174	1.00	7.84
ATOM	710	O ARG	99	68.179	49.159	31.118	1.00	8.53
ATOM	711	N VAL	100	66.528	50.307	30.136	1.00	5.56
ATOM	712	CA VAL	100	66.670	49.664	28.852	1.00	5.54
ATOM	713	CB VAL	100	65.321	49.097	28.397	1.00	8.61
ATOM	714	CG1 VAL	100	65.446	48.467	27.008	1.00	7.63
ATOM	715	CG2 VAL	100	64.821	48.100	29.419	1.00	7.70
ATOM	716	C VAL	100	67.146	50.745	27.877	1.00	6.61
ATOM	717	O VAL	100	66.556	51.831	27.819	1.00	3.63
ATOM	718	N THR	101	68.236	50.490	27.156	1.00	7.98
ATOM	719	CA THR	101	68.768	51.483	25.193	1.00	10.18
ATOM	720	CB THR	101	70.000	52.277	26.748	1.00	8.43
ATOM	721	CG1 THR	101	70.526	51.629	27.908	1.00	13.91
ATOM	722	CG2 THR	101	69.603	52.663	27.148	1.00	11.20
ATOM	723	C THR	101	69.115	50.926	24.792	1.00	11.66
ATOM	724	O THR	101	69.483	49.758	24.645	1.00	11.61
ATOM	725	N ALA	102	68.915	51.752	23.767	1.00	12.50
ATOM	726	CA ALA	102	69.216	51.369	22.386	1.00	14.07
ATOM	727	CB ALA	102	68.735	52.465	21.399	1.00	14.73
ATOM	728	C ALA	102	70.721	51.154	22.249	1.00	13.24
ATOM	729	O ALA	102	71.511	51.752	23.012	1.00	12.22
ATOM	730	N ALA	103	71.111	50.332	21.270	1.00	12.73
ATOM	731	CA ALA	103	72.520	50.004	21.021	1.00	13.74
ATOM	732	CB ALA	103	72.631	48.712	20.183	1.00	15.06
ATOM	733	C ALA	103	73.250	51.173	20.338	1.00	14.07
ATOM	734	O ALA	103	73.958	51.013	19.345	1.00	16.53
ATOM	735	N SER	104	73.105	52.341	20.931	1.00	12.51
ATOM	736	CA SER	104	73.673	53.569	20.440	1.00	10.25
ATOM	737	CB SER	104	72.834	54.066	19.266	1.00	9.41
ATOM	738	OG SER	104	71.434	54.033	19.565	1.00	8.47
ATOM	739	C SER	104	73.507	54.528	21.600	1.00	11.58
ATOM	740	O SER	104	73.557	55.746	21.412	1.00	11.80
ATOM	741	N GLY	105	73.187	53.964	22.770	1.00	11.41
ATOM	742	CA GLY	105	73.002	54.747	22.976	1.00	12.64
ATOM	743	C GLY	105	71.737	55.568	23.980	1.00	13.51
ATOM	744	O GLY	105	71.507	56.335	24.921	1.00	15.64
ATOM	745	N ALA	106	70.929	55.433	22.930	1.00	12.54
ATOM	746	CA ALA	106	69.668	56.166	22.837	1.00	11.65
ATOM	747	CB ALA	106	69.068	56.040	21.444	1.00	12.77
ATOM	748	C ALA	106	68.752	55.553	23.884	1.00	11.28
ATOM	749	O ALA	106	68.501	54.338	23.899	1.00	10.70
ATOM	750	N PRO	107	68.239	56.392	24.779	1.00	8.60
ATOM	751	CD PRO	107	68.390	57.855	24.686	1.00	9.28
ATOM	752	CA PRO	107	67.354	56.019	25.882	1.00	7.77
ATOM	753	CB PRO	107	67.282	57.314	26.683	1.00	8.42
ATOM	754	CG PRO	107	67.302	58.358	25.605	1.00	9.15
ATOM	755	C PRO	107	65.964	55.459	25.552	1.00	7.66
ATOM	756	O PRO	107	65.224	56.048	24.781	1.00	8.78
ATOM	757	N ARG	108	65.595	54.353	25.196	1.00	7.20
ATOM	758	CA ARG	108	64.290	53.751	25.990	1.00	4.63
ATOM	759	CB ARG	108	64.439	52.411	25.258	1.00	7.43
ATOM	760	CG ARG	108	63.168	51.902	24.695	1.00	10.88
ATOM	761	CD ARG	108	62.782	52.688	23.460	1.00	14.12
ATOM	762	NE ARG	108	61.461	52.318	22.964	1.00	16.25
ATOM	763	CZ ARG	108	61.086	51.084	22.650	1.00	15.01
ATOM	764	NH1 ARG	108	61.917	50.067	22.764	1.00	18.31
ATOM	765	NH2 ARG	108	59.858	50.867	22.236	1.00	19.47
ATOM	766	C ARG	108	63.455	53.624	27.253	1.00	5.36
ATOM	767	O ARG	108	62.420	54.259	27.404	1.00	6.86
ATOM	768	N TYR	109	63.882	52.827	28.263	1.00	6.12
ATOM	769	CA TYR	109	63.102	52.711	29.509	1.00	6.72
ATOM	770	CB TYR	109	62.419	51.350	29.631	1.00	7.62
ATOM	771	CG TYR	109	61.455	51.024	28.544	1.00	8.20
ATOM	772	CD1 TYR	109	61.775	50.089	27.565	1.00	11.38

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ATOM	773	CE1	TYR	109	60.897	49.788	26.557	1.00	12.39	4
ATOM	774	CD2	TYR	109	60.230	51.642	28.480	1.00	10.61	6
ATOM	775	CE2	TYR	109	59.337	51.347	27.476	1.00	12.42	5
ATOM	776	CZ	TYR	109	59.670	50.421	26.511	1.00	12.48	6
ATOM	777	OH	TYR	109	58.777	50.152	25.481	1.00	14.44	2
ATOM	778	C	TYR	109	63.911	52.909	30.774	1.00	8.52	5
ATOM	779	O	TYR	109	65.124	52.737	30.794	1.00	9.59	2
ATOM	780	N	HIS	110	63.198	53.259	31.835	1.00	10.99	7
ATOM	781	CA	HIS	110	63.760	53.467	33.174	1.00	14.45	5
ATOM	782	CB	HIS	110	64.468	54.830	33.296	1.00	16.07	5
ATOM	783	CG	HIS	110	65.167	55.029	34.613	1.00	21.12	6
ATOM	784	CD2	HIS	110	66.383	54.616	35.048	1.00	21.71	5
ATOM	785	ND1	HIS	110	64.623	55.764	35.652	1.00	24.07	7
ATOM	786	CE1	HIS	110	65.476	55.803	36.662	1.00	23.40	6
ATOM	787	NE2	HIS	110	66.553	55.114	36.321	1.00	22.60	7
ATOM	788	C	HIS	110	62.628	53.380	34.214	1.00	12.21	6
ATOM	789	O	HIS	110	61.740	54.224	34.240	1.00	13.06	8
ATOM	790	N	ARG	111	62.693	52.361	35.062	1.00	11.08	7
ATOM	791	CA	ARG	111	61.716	52.116	36.112	1.00	10.30	6
ATOM	792	CB	ARG	111	60.878	50.881	35.742	1.00	9.90	6
ATOM	793	CG	ARG	111	59.700	50.590	36.641	1.00	8.05	6
ATOM	794	CD	ARG	111	58.370	50.465	35.862	1.00	8.40	5
ATOM	795	NE	ARG	111	57.828	49.099	35.783	1.00	8.93	7
ATOM	796	CZ	ARG	111	57.096	48.521	36.730	1.00	8.80	5
ATOM	797	NH1	ARG	111	56.822	49.182	37.840	1.00	10.13	7
ATOM	798	NH2	ARG	111	56.585	47.308	36.550	1.00	10.84	7
ATOM	799	C	ARG	111	62.546	51.850	37.369	1.00	11.27	5
ATOM	800	O	ARG	111	63.776	51.808	37.306	1.00	13.11	3
ATOM	801	N	VAL	112	61.877	51.758	39.510	1.00	11.56	7
ATOM	802	CA	VAL	112	62.493	51.471	39.822	1.00	11.15	6
ATOM	803	CB	VAL	112	62.882	52.803	40.601	1.00	12.50	5
ATOM	804	CG1	VAL	112	63.003	52.545	42.094	1.00	13.08	6
ATOM	805	CG2	VAL	112	64.235	53.354	40.093	1.00	12.31	6
ATOM	806	C	VAL	112	61.398	50.668	40.542	1.00	7.77	5
ATOM	807	O	VAL	112	60.268	51.105	40.581	1.00	8.50	3
ATOM	808	N	ILE	113	61.709	49.480	41.049	1.00	5.20	7
ATOM	809	CA	ILE	113	60.692	48.638	41.686	1.00	6.80	6
ATOM	810	CB	ILE	113	60.223	47.527	40.688	1.00	5.60	6
ATOM	811	CG2	ILE	113	59.680	48.130	39.426	1.00	6.45	5
ATOM	812	CG1	ILE	113	61.396	46.623	40.315	1.00	7.39	5
ATOM	813	CD1	ILE	113	61.012	45.471	39.468	1.00	9.87	6
ATOM	814	C	ILE	113	61.105	47.931	43.001	1.00	7.16	5
ATOM	815	O	ILE	113	62.141	48.234	43.572	1.00	9.02	5
ATOM	816	N	HIS	114	60.267	47.000	43.463	1.00	2.78	7
ATOM	817	CA	HIS	114	60.503	46.187	44.645	1.00	2.00	5
ATOM	818	CB	HIS	114	59.793	46.758	45.860	1.00	2.00	5
ATOM	819	CG	HIS	114	60.554	47.827	46.555	1.00	2.00	5
ATOM	820	CD2	HIS	114	61.337	47.787	47.652	1.00	4.22	5
ATOM	821	ND1	HIS	114	60.589	49.130	46.106	1.00	4.03	7
ATOM	822	CE1	HIS	114	61.368	49.850	46.891	1.00	2.34	5
ATOM	823	NE2	HIS	114	61.835	49.057	47.838	1.00	8.31	7
ATOM	824	C	HIS	114	59.907	44.830	44.330	1.00	2.00	5
ATOM	825	O	HIS	114	58.705	44.688	44.221	1.00	2.00	5
ATOM	826	N	ILE	115	60.741	43.922	44.201	1.00	2.50	7
ATOM	827	CA	ILE	115	60.261	42.495	43.871	1.00	2.00	5
ATOM	828	CB	ILE	115	61.439	41.480	43.883	1.00	3.64	5
ATOM	829	CG2	ILE	115	60.953	40.049	43.984	1.00	4.23	5
ATOM	830	CG1	ILE	115	62.333	41.672	42.650	1.00	2.00	5
ATOM	831	CD1	ILE	115	63.731	42.190	42.966	1.00	2.23	5
ATOM	832	C	ILE	115	59.107	42.012	44.751	1.00	3.56	5
ATOM	833	O	ILE	115	58.294	41.217	44.302	1.00	6.91	5
ATOM	834	N	ASN	116	59.012	42.492	45.985	1.00	4.63	5
ATOM	835	CA	ASN	116	57.936	42.066	46.895	1.00	5.21	5
ATOM	836	CB	ASN	116	58.317	42.342	43.370	1.00	5.33	5
ATOM	837	CG	ASN	116	58.582	43.223	43.655	1.00	5.94	5
ATOM	838	OD1	ASN	116	59.470	44.421	48.070	1.00	8.06	5
ATOM	839	ND2	ASN	116	57.806	44.414	47.551	1.00	8.46	7
ATOM	840	C	ASN	116	56.589	42.723	46.547	1.00	5.92	5
ATOM	841	O	ASN	116	55.512	42.233	46.879	1.00	4.52	5
ATOM	842	N	GLU	117	56.664	43.852	45.841	1.00	8.36	5
ATOM	843	CA	GLU	117	55.480	44.614	45.436	1.00	7.65	5
ATOM	844	CB	GLU	117	55.732	46.113	45.534	1.00	6.11	5
ATOM	845	CG	GLU	117	55.958	46.606	46.937	1.00	12.42	5
ATOM	846	CD	GLU	117	56.160	48.090	47.002	1.00	15.01	5
ATOM	847	OE1	GLU	117	56.648	48.601	48.056	1.00	18.35	5
ATOM	848	OE2	GLU	117	55.816	48.757	46.002	1.00	15.71	5
ATOM	849	C	GLU	117	55.116	44.321	44.025	1.00	6.25	5
ATOM	850	O	GLU	117	54.446	45.120	43.426	1.00	9.90	5

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ATOM  851 N VAL 118 55.477 43.151 43.523 1.00 3.55 7
ATOM  852 CA VAL 118 55.226 42.839 42.137 1.00 2.91 5
ATOM  853 CB VAL 118 56.373 43.488 41.261 1.00 2.00 5
ATOM  854 CG1 VAL 118 57.484 42.519 40.942 1.00 2.85 5
ATOM  855 CG2 VAL 118 55.828 44.165 40.062 1.00 2.00 5
ATOM  856 C VAL 118 55.060 41.334 41.948 1.00 2.18 5
ATOM  857 O VAL 118 55.453 40.755 40.936 1.00 3.50 5
ATOM  858 N VAL 119 54.404 40.716 42.919 1.00 2.75 7
ATOM  859 CA VAL 119 54.155 39.276 42.896 1.00 3.05 5
ATOM  860 CB VAL 119 53.778 38.736 44.305 1.00 2.45 5
ATOM  861 CG1 VAL 119 53.749 37.267 44.292 1.00 2.00 5
ATOM  862 CG2 VAL 119 54.735 39.231 45.352 1.00 2.00 5
ATOM  863 C VAL 119 52.998 38.960 41.945 1.00 2.00 5
ATOM  864 O VAL 119 52.007 39.674 41.932 1.00 2.00 5
ATOM  865 N LEU 120 53.171 37.919 41.132 1.00 3.02 7
ATOM  866 CA LEU 120 52.175 37.411 40.174 1.00 2.95 5
ATOM  867 CB LEU 120 52.446 37.894 38.745 1.00 5.65 5
ATOM  868 CG LEU 120 51.496 37.332 37.674 1.00 11.07 5
ATOM  869 CD1 LEU 120 50.125 37.938 37.790 1.00 9.95 5
ATOM  870 CD2 LEU 120 52.053 37.605 36.306 1.00 11.67 5
ATOM  871 C LEU 120 52.289 35.887 40.262 1.00 2.40 5
ATOM  872 O LEU 120 52.985 35.241 39.487 1.00 2.00 5
ATOM  873 N LEU 121 51.600 35.340 41.250 1.00 2.39 7
ATOM  874 CA LEU 121 51.629 33.924 41.552 1.00 2.77 5
ATOM  875 CB LEU 121 51.063 33.689 42.964 1.00 4.57 5
ATOM  876 CG LEU 121 52.050 33.227 44.062 1.00 10.24 5
ATOM  877 CD1 LEU 121 52.939 32.076 43.550 1.00 14.57 5
ATOM  878 CD2 LEU 121 52.944 34.328 44.501 1.00 9.42 5
ATOM  879 C LEU 121 50.974 32.995 40.534 1.00 5.41 5
ATOM  880 O LEU 121 50.256 33.420 39.634 1.00 7.90 5
ATOM  881 N ASP 122 51.279 31.709 40.672 1.00 8.57 7
ATOM  882 CA ASP 122 50.687 30.726 39.782 1.00 6.90 5
ATOM  883 CB ASP 122 51.493 29.421 39.773 1.00 7.76 5
ATOM  884 CG ASP 122 52.701 29.437 38.795 1.00 9.54 5
ATOM  885 OD1 ASP 122 52.927 30.429 38.066 1.00 9.98 5
ATOM  886 OD2 ASP 122 53.411 28.405 38.748 1.00 10.20 5
ATOM  887 C ASP 122 49.292 30.494 40.343 1.00 7.04 5
ATOM  888 O ASP 122 48.957 30.954 41.453 1.00 5.44 5
ATOM  889 N ALA 123 48.464 29.813 39.568 1.00 6.22 7
ATOM  890 CA ALA 123 47.107 29.562 40.010 1.00 4.76 5
ATOM  891 CB ALA 123 46.187 29.374 38.839 1.00 2.00 5
ATOM  892 C ALA 123 46.981 28.398 40.954 1.00 3.93 5
ATOM  893 O ALA 123 47.826 27.484 40.971 1.00 5.37 5
ATOM  894 N PRO 124 45.979 28.490 41.846 1.00 2.51 7
ATOM  895 CD PRO 124 45.216 29.736 42.096 1.00 2.90 5
ATOM  896 CA PRO 124 45.652 27.478 42.845 1.00 2.91 5
ATOM  897 CB PRO 124 44.362 28.022 43.436 1.00 2.00 5
ATOM  898 CG PRO 124 44.602 29.485 43.432 1.00 2.00 5
ATOM  899 C PRO 124 45.451 26.111 42.172 1.00 2.00 5
ATOM  900 O PRO 124 45.289 26.022 40.966 1.00 2.00 5
ATOM  901 N VAL 125 45.524 25.042 42.944 1.00 2.21 7
ATOM  902 CA VAL 125 45.345 23.715 42.381 1.00 4.06 5
ATOM  903 CB VAL 125 46.724 23.006 42.025 1.00 2.00 5
ATOM  904 CG1 VAL 125 47.474 23.806 40.974 1.00 2.00 5
ATOM  905 CG2 VAL 125 47.584 22.776 43.256 1.00 2.00 5
ATOM  906 C VAL 125 44.436 22.838 43.267 1.00 5.51 5
ATOM  907 O VAL 125 44.002 23.281 44.316 1.00 6.23 5
ATOM  908 N GLY 126 44.068 21.661 42.768 1.00 5.29 7
ATOM  909 CA GLY 126 43.230 20.735 43.494 1.00 4.11 5
ATOM  910 C GLY 126 41.939 21.283 44.035 1.00 5.54 5
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ATOM  912 N LEU 127 41.248 22.112 43.268 1.00 5.53 7
ATOM  913 CA LEU 127 39.971 22.667 43.718 1.00 7.27 5
ATOM  914 CB LEU 127 39.594 23.949 42.935 1.00 3.72 5
ATOM  915 CG LEU 127 38.175 24.573 43.071 1.00 11.14 5
ATOM  916 CD1 LEU 127 37.954 25.322 44.424 1.00 7.43 5
ATOM  917 CD2 LEU 127 37.942 25.515 41.892 1.00 10.21 5
ATOM  918 C LEU 127 38.846 21.623 43.612 1.00 6.98 5
ATOM  919 O LEU 127 38.585 21.083 42.538 1.00 6.55 5
ATOM  920 N VAL 128 38.177 21.369 44.737 1.00 7.13 7
ATOM  921 CA VAL 128 37.087 20.406 44.815 1.00 6.92 5
ATOM  922 CB VAL 128 37.485 19.147 45.616 1.00 7.07 5
ATOM  923 CG1 VAL 128 37.999 18.089 44.701 1.00 7.21 5
ATOM  924 CG2 VAL 128 38.521 19.477 46.659 1.00 9.12 5
ATOM  925 C VAL 128 35.862 21.001 45.470 1.00 5.27 5
ATOM  926 O VAL 126 35.973 21.795 46.374 1.00 6.57 5
ATOM  927 N ALA 129 34.691 20.574 45.031 1.00 7.13 7
ATOM  928 CA ALA 129 33.430 21.061 45.579 1.00 6.61 5

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ATOM	929	CB	ALA	129	32.585	21.680	44.477	1.00	4.36	6
ATOM	930	C	ALA	129	32.693	19.876	46.202	1.00	9.11	6
ATOM	931	O	ALA	129	32.730	18.760	45.655	1.00	9.32	3
ATOM	932	N	ARG	130	32.018	20.106	47.329	1.00	9.76	7
ATOM	933	CA	ARG	130	31.288	19.020	47.990	1.00	10.55	6
ATOM	934	CB	ARG	130	32.220	18.310	48.967	1.00	11.88	6
ATOM	935	CG	ARG	130	31.765	16.979	49.486	1.00	11.87	6
ATOM	936	CD	ARG	130	32.108	16.871	50.963	1.00	15.67	6
ATOM	937	NE	ARG	130	33.351	17.567	51.252	1.00	15.76	7
ATOM	938	CZ	ARG	130	33.669	18.135	52.414	1.00	20.46	6
ATOM	939	NH1	ARG	130	32.818	18.092	53.449	1.00	18.08	7
ATOM	940	NH2	ARG	130	34.840	18.791	52.514	1.00	21.04	7
ATOM	941	C	ARG	130	30.028	19.479	48.721	1.00	10.90	6
ATOM	942	O	ARG	130	29.932	20.593	49.250	1.00	10.77	8
ATOM	943	N	LEU	131	29.065	18.582	48.792	1.00	12.00	7
ATOM	944	CA	LEU	131	27.813	18.909	49.460	1.00	13.66	6
ATOM	945	CB	LEU	131	26.640	18.313	48.688	1.00	12.73	6
ATOM	946	CG	LEU	131	25.301	18.517	49.353	1.00	11.96	6
ATOM	947	CD1	LEU	131	25.035	20.002	49.487	1.00	10.47	6
ATOM	948	CD2	LEU	131	24.252	17.783	48.531	1.00	11.69	6
ATOM	949	C	LEU	131	27.799	18.409	50.892	1.00	13.46	6
ATOM	950	O	LEU	131	27.702	17.204	51.128	1.00	12.81	8
ATOM	951	N	ALA	132	27.968	19.328	51.834	1.00	14.88	7
ATOM	952	CA	ALA	132	27.964	18.982	53.249	1.00	16.22	6
ATOM	953	CB	ALA	132	28.272	20.228	54.122	1.00	14.97	6
ATOM	954	C	ALA	132	26.638	18.324	53.656	1.00	16.57	6
ATOM	955	O	ALA	132	25.719	19.000	54.109	1.00	16.97	6
ATOM	956	N	ASP	133	26.553	17.009	53.411	1.00	20.15	7
ATOM	957	CA	ASP	133	25.397	16.156	53.729	1.00	22.27	6
ATOM	958	CB	ASP	133	25.868	14.755	54.193	1.00	23.23	6
ATOM	959	CG	ASP	133	26.187	12.783	53.024	1.00	25.72	6
ATOM	960	OD1	ASP	133	25.704	14.012	51.871	1.00	26.91	3
ATOM	961	OD2	ASP	133	26.894	12.758	53.284	1.00	25.03	3
ATOM	962	C	ASP	133	24.655	16.814	54.885	1.00	22.10	6
ATOM	963	O	ASP	133	23.575	17.415	54.715	1.00	24.05	8
ATOM	964	N	GLU	134	25.310	16.802	56.037	1.00	19.91	7
ATOM	965	CA	GLU	134	24.742	17.410	57.211	1.00	18.60	6
ATOM	966	CB	GLU	134	25.478	16.953	58.482	1.00	17.36	6
ATOM	967	CG	GLU	134	26.589	15.897	58.287	1.00	17.83	6
ATOM	968	CD	GLU	134	28.003	16.514	58.153	1.00	20.37	6
ATOM	969	OE1	GLU	134	28.980	15.726	58.020	1.00	19.82	8
ATOM	970	OE2	GLU	134	28.136	17.775	58.183	1.00	18.81	3
ATOM	971	C	GLU	134	24.784	18.933	57.068	1.00	17.19	6
ATOM	972	O	GLU	134	25.842	19.534	57.197	1.00	18.37	3
ATOM	973	N	SER	135	23.648	19.496	56.657	1.00	16.42	7
ATOM	974	CA	SER	135	23.375	20.938	56.510	1.00	17.66	6
ATOM	975	CB	SER	135	24.435	21.857	57.166	1.00	17.67	6
ATOM	976	OG	SER	135	25.623	21.981	56.400	1.00	19.35	3
ATOM	977	C	SER	135	22.990	21.443	55.124	1.00	18.19	6
ATOM	978	O	SER	135	22.366	22.501	54.991	1.00	17.96	8
ATOM	979	N	GLY	136	23.287	20.665	54.095	1.00	19.82	7
ATOM	980	CA	GLY	136	22.945	21.109	52.753	1.00	21.54	6
ATOM	981	C	GLY	136	23.765	22.335	52.372	1.00	22.07	6
ATOM	982	O	GLY	136	23.225	23.345	51.910	1.00	22.69	3
ATOM	983	N	HIS	137	25.071	22.258	52.622	1.00	21.69	7
ATOM	984	CA	HIS	137	25.992	23.332	52.301	1.00	19.69	6
ATOM	985	CB	HIS	137	26.594	22.884	53.590	1.00	22.11	6
ATOM	986	CG	HIS	137	25.768	24.968	54.204	1.00	25.43	6
ATOM	987	CD2	HIS	137	26.049	25.862	55.183	1.00	27.18	6
ATOM	988	ND1	HIS	137	24.484	25.256	53.777	1.00	26.89	7
ATOM	989	CE1	HIS	137	24.014	26.287	54.465	1.00	26.67	6
ATOM	990	NE2	HIS	137	24.944	26.674	55.325	1.00	26.59	7
ATOM	991	C	HIS	137	27.081	22.863	51.329	1.00	19.46	6
ATOM	992	O	HIS	137	27.428	21.666	51.301	1.00	20.08	3
ATOM	993	N	VAL	138	27.547	22.771	50.468	1.00	16.09	7
ATOM	994	CA	VAL	138	28.598	23.427	49.526	1.00	12.40	6
ATOM	995	CB	VAL	138	28.391	24.107	48.143	1.00	12.43	6
ATOM	996	CG1	VAL	138	29.725	24.286	47.390	1.00	10.78	6
ATOM	997	CG2	VAL	138	27.444	23.258	47.290	1.00	12.93	6
ATOM	998	C	VAL	138	29.891	23.877	50.156	1.00	11.10	3
ATOM	999	O	VAL	138	29.960	24.376	50.705	1.00	11.62	3
ATOM	1000	N	VAL	139	30.872	22.982	50.171	1.00	9.36	7
ATOM	1001	CA	VAL	139	32.194	23.268	50.724	1.00	10.38	3
ATOM	1002	CB	VAL	139	32.539	22.371	51.949	1.00	6.78	6
ATOM	1003	CG1	VAL	139	33.781	22.877	52.620	1.00	7.80	6
ATOM	1004	CG2	VAL	139	31.415	22.393	52.946	1.00	6.80	6
ATOM	1005	C	VAL	139	33.249	23.095	49.615	1.00	10.04	6
ATOM	1006	O	VAL	139	33.333	22.026	48.961	1.00	10.34	3

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ATOM	1007	N	LEU	140	33.975	24.194	49.372	1.00	3.25	7	
ATOM	1008	CA	LEU	140	35.027	24.306	43.384	1.00	6.26	5	
ATOM	1009	CB	LEU	140	34.986	25.673	47.761	1.00	2.05	5	
ATOM	1010	CG	LEU	140	33.726	25.968	47.000	1.00	2.00	5	
ATOM	1011	CD1	LEU	140	33.806	27.395	46.505	1.00	2.00	5	
ATOM	1012	CD2	LEU	140	33.594	24.972	45.869	1.00	2.00	5	
ATOM	1013	C	LEU	140	36.354	24.170	49.069	1.00	3.88	5	
ATOM	1014	O	LEU	140	36.566	24.774	50.115	1.00	10.60	5	
ATOM	1015	N	ARG	141	37.278	23.481	48.409	1.00	11.34	7	
ATOM	1016	CA	ARG	141	38.618	23.235	48.929	1.00	12.76	5	
ATOM	1017	CB	ARG	141	38.682	21.805	49.446	1.00	16.99	5	
ATOM	1018	CG	ARG	141	39.347	21.645	50.793	1.00	21.35	5	
ATOM	1019	CD	ARG	141	40.849	21.410	50.697	1.00	24.13	6	
ATOM	1020	NE	ARG	141	41.431	21.433	52.042	1.00	29.12	7	
ATOM	1021	CZ	ARG	141	42.344	22.314	52.482	1.00	30.00	6	
ATOM	1022	NH1	ARG	141	42.821	23.266	51.673	1.00	30.75	7	
ATOM	1023	NH2	ARG	141	42.727	22.282	53.773	1.00	29.95	7	
ATOM	1024	C	ARG	141	39.632	23.383	47.804	1.00	13.10	6	
ATOM	1025	O	ARG	141	39.289	23.227	46.639	1.00	13.55	5	
ATOM	1026	N	TRP	142	40.871	23.715	48.154	1.00	11.10	7	
ATOM	1027	CA	TRP	142	41.941	23.846	47.182	1.00	6.61	5	
ATOM	1028	CB	TRP	142	41.754	25.107	46.354	1.00	6.92	5	
ATOM	1029	CG	TRP	142	41.661	26.356	47.155	1.00	9.55	5	
ATOM	1030	CD2	TRP	142	40.482	26.905	47.749	1.00	9.85	5	
ATOM	1031	CE2	TRP	142	40.852	28.094	48.397	1.00	9.31	5	
ATOM	1032	CE3	TRP	142	39.145	26.508	47.788	1.00	10.67	5	
ATOM	1033	CD1	TRP	142	42.671	27.216	47.456	1.00	10.90	5	
ATOM	1034	NE1	TRP	142	42.196	28.267	48.209	1.00	11.52	7	
ATOM	1035	CZ2	TRP	142	39.937	28.885	49.072	1.00	11.31	5	
ATOM	1036	CZ3	TRP	142	38.245	27.296	48.454	1.00	11.65	5	
ATOM	1037	CH2	TRP	142	38.645	28.474	49.089	1.00	9.80	5	
ATOM	1038	C	TRP	142	43.288	23.857	47.877	1.00	5.00	6	
ATOM	1039	O	TRP	142	43.380	23.703	49.076	1.00	6.66	3	
ATOM	1040	N	LEU	143	44.349	23.995	47.109	1.00	5.47	7	
ATOM	1041	CA	LEU	143	45.700	24.039	47.656	1.00	3.56	6	
ATOM	1042	CB	LEU	143	46.520	22.876	47.123	1.00	2.35	5	
ATOM	1043	CG	LEU	143	46.031	21.474	47.408	1.00	2.00	6	
ATOM	1044	CD1	LEU	143	46.832	20.483	46.601	1.00	2.00	6	
ATOM	1045	CD2	LEU	143	46.182	21.223	48.862	1.00	2.00	5	
ATOM	1046	C	LEU	143	46.310	25.326	47.158	1.00	2.00	6	
ATOM	1047	O	LEU	143	45.765	25.970	46.274	1.00	4.81	3	
ATOM	1048	N	PRO	144	47.411	25.759	47.762	1.00	2.00	7	
ATOM	1049	CD	PRO	144	48.002	25.327	49.030	1.00	2.00	5	
ATOM	1050	CA	PRO	144	48.027	26.996	47.295	1.00	2.00	5	
ATOM	1051	CB	PRO	144	48.955	27.359	48.445	1.00	2.00	5	
ATOM	1052	CG	PRO	144	48.442	26.605	49.601	1.00	2.00	5	
ATOM	1053	C	PRO	144	48.821	26.750	46.011	1.00	2.00	5	
ATOM	1054	O	PRO	144	48.999	25.611	45.560	1.00	2.00	3	
ATOM	1055	N	PRO	145	49.249	27.823	45.342	1.00	2.00	7	
ATOM	1056	CD	PRO	145	49.058	29.249	45.645	1.00	2.00	5	
ATOM	1057	CA	PRO	145	50.022	27.643	44.113	1.00	2.72	5	
ATOM	1058	CB	PRO	145	50.532	29.053	43.839	1.00	2.80	5	
ATOM	1059	CG	PRO	145	49.457	29.828	44.372	1.00	2.95	5	
ATOM	1060	C	PRO	145	51.178	26.696	44.455	1.00	4.71	5	
ATOM	1061	O	PRO	145	51.875	26.899	45.448	1.00	3.80	5	
ATOM	1062	N	PRO	146	51.396	25.652	43.639	1.00	9.22	7	
ATOM	1063	CD	PRO	146	50.738	25.412	42.347	1.00	5.90	5	
ATOM	1064	CA	PRO	146	52.462	24.665	43.857	1.00	6.83	5	
ATOM	1065	CB	PRO	146	52.358	23.778	42.622	1.00	7.88	5	
ATOM	1066	CG	PRO	146	50.972	23.951	42.167	1.00	5.28	5	
ATOM	1067	C	PRO	146	53.863	25.273	43.967	1.00	9.28	5	
ATOM	1068	O	PRO	146	54.272	26.087	43.125	1.00	10.56	5	
ATOM	1069	N	GLU	147	54.604	24.825	44.975	1.00	10.34	7	
ATOM	1070	CA	GLU	147	55.959	25.281	45.248	1.00	9.65	5	
ATOM	1071	CB	GLU	147	56.894	24.958	44.077	1.00	9.95	5	
ATOM	1072	CG	GLU	147	56.733	23.566	43.456	1.00	18.10	5	
ATOM	1073	CD	GLU	147	57.477	22.401	44.166	1.00	22.76	5	
ATOM	1074	OE1	GLU	147	58.335	22.639	45.061	1.00	25.12	5	
ATOM	1075	OE2	GLU	147	57.207	21.215	43.789	1.00	23.73	5	
ATOM	1076	C	GLU	147	56.052	26.773	45.624	1.00	10.12	5	
ATOM	1077	O	GLU	147	57.099	27.403	45.453	1.00	12.66	5	
ATOM	1078	N	THR	148	54.975	27.364	45.124	1.00	10.44	7	
ATOM	1079	CA	THR	148	55.048	28.776	45.541	1.00	7.37	5	
ATOM	1080	CB	THR	148	53.778	29.551	45.178	1.00	5.61	5	
ATOM	1081	OG1	THR	148	53.589	29.464	44.765	1.00	4.74	5	
ATOM	1082	OG2	THR	148	53.881	31.014	45.621	1.00	2.30	5	
ATOM	1083	C	THR	148	55.272	28.818	43.048	1.00	5.00	5	
ATOM	1084	O	THR	148	54.609	28.080	43.789	1.00	4.53	5	

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ATOM	1085	N	PRO	149	56.279	29.605	48.503	1.00	7.63		
ATOM	1086	CD	PRO	149	57.156	30.457	47.666	1.00	4.62		
ATOM	1087	CA	PRO	149	56.623	29.757	49.926	1.00	5.20		
ATOM	1088	CB	PRO	149	58.074	30.190	49.860	1.00	2.62		
ATOM	1089	CG	PRO	149	58.050	31.144	48.698	1.00	2.00		
ATOM	1090	C	PRO	149	55.742	30.869	50.498	1.00	7.00		
ATOM	1091	O	PRO	149	55.080	31.600	49.737	1.00	10.83		
ATOM	1092	N	MET	150	55.727	31.012	51.814	1.00	7.26		
ATOM	1093	CA	MET	150	54.916	32.048	52.464	1.00	5.41		
ATOM	1094	CB	MET	150	55.415	33.469	52.109	1.00	5.16		
ATOM	1095	CG	MET	150	56.864	33.812	52.512	1.00	2.00		
ATOM	1096	SD	MET	150	57.164	33.978	54.292	1.00	8.51		
ATOM	1097	CE	MET	150	57.009	35.706	54.546	1.00	2.48		
ATOM	1098	C	MET	150	53.411	31.927	52.169	1.00	5.15		
ATOM	1099	O	MET	150	52.749	32.952	52.002	1.00	4.08		
ATOM	1100	N	THR	151	52.878	30.696	52.239	1.00	3.72		
ATOM	1101	CA	THR	151	51.464	30.405	51.963	1.00	3.59		
ATOM	1102	CB	THR	151	51.157	28.902	51.799	1.00	2.22		
ATOM	1103	OG1	THR	151	51.381	28.183	52.955	1.00	8.69		
ATOM	1104	CG2	THR	151	51.821	28.347	50.609	1.00	3.84		
ATOM	1105	C	THR	151	50.402	30.920	52.922	1.00	5.68		
ATOM	1106	O	THR	151	49.218	30.919	52.583	1.00	7.24		
ATOM	1107	N	SER	152	50.774	31.331	54.123	1.00	6.42		
ATOM	1108	CA	SER	152	49.755	31.831	55.041	1.00	6.44		
ATOM	1109	CB	SER	152	50.178	31.598	56.476	1.00	6.46		
ATOM	1110	OG	SER	152	51.027	32.645	56.893	1.00	5.38		
ATOM	1111	C	SER	152	49.563	33.321	54.842	1.00	7.14		
ATOM	1112	O	SER	152	48.982	33.976	55.687	1.00	10.30		
ATOM	1113	N	HIS	153	50.148	33.866	53.780	1.00	7.23		
ATOM	1114	CA	HIS	153	50.070	35.291	53.485	1.00	5.69		
ATOM	1115	CB	HIS	153	51.479	35.883	53.275	1.00	4.92		
ATOM	1116	CG	HIS	153	52.310	35.975	54.526	1.00	4.89		
ATOM	1117	CD2	HIS	153	52.810	37.048	55.182	1.00	3.84		
ATOM	1118	ND1	HIS	153	52.781	34.868	55.197	1.00	6.02		
ATOM	1119	CE1	HIS	153	53.540	35.254	56.204	1.00	3.19		
ATOM	1120	NE2	HIS	153	53.573	36.570	56.215	1.00	2.00		
ATOM	1121	C	HIS	153	49.275	35.491	52.227	1.00	2.54		
ATOM	1122	O	HIS	153	49.013	36.614	51.811	1.00	6.78		
ATOM	1123	N	ILE	154	48.937	34.385	51.603	1.00	2.00		
ATOM	1124	CA	ILE	154	48.201	34.412	50.377	1.00	2.00		
ATOM	1125	CB	ILE	154	48.493	33.116	49.523	1.00	2.00		
ATOM	1126	CG2	ILE	154	47.906	33.208	48.126	1.00	2.06		
ATOM	1127	CG1	ILE	154	49.982	32.883	49.376	1.00	2.00		
ATOM	1128	CD1	ILE	154	50.301	31.727	48.512	1.00	2.00		
ATOM	1129	C	ILE	154	46.702	34.532	50.669	1.00	2.05		
ATOM	1130	O	ILE	154	46.165	33.897	51.564	1.00	2.00		
ATOM	1131	N	ARG	155	46.068	35.391	49.885	1.00	4.56		
ATOM	1132	CA	ARG	155	44.638	35.649	49.910	1.00	5.20		
ATOM	1133	CB	ARG	155	44.372	37.149	49.818	1.00	5.20		
ATOM	1134	CG	ARG	155	44.596	37.920	51.094	1.00	8.42		
ATOM	1135	CD	ARG	155	44.382	39.399	50.848	1.00	14.35		
ATOM	1136	NE	ARG	155	44.206	40.104	52.119	1.00	24.48		
ATOM	1137	CZ	ARG	155	44.822	41.229	52.496	1.00	27.55		
ATOM	1138	NH1	ARG	155	45.718	41.848	51.699	1.00	25.45		
ATOM	1139	NH2	ARG	155	44.600	41.707	53.725	1.00	28.94		
ATOM	1140	C	ARG	155	44.067	34.962	48.668	1.00	5.00		
ATOM	1141	O	ARG	155	44.800	34.760	47.678	1.00	5.12		
ATOM	1142	N	TYR	156	42.782	34.596	48.739	1.00	5.08		
ATOM	1143	CA	TYR	156	42.077	33.927	47.651	1.00	5.24		
ATOM	1144	CB	TYR	156	41.774	32.474	48.011	1.00	5.18		
ATOM	1145	CG	TYR	156	42.978	31.665	48.339	1.00	10.56		
ATOM	1146	CD1	TYR	156	43.447	31.591	49.651	1.00	13.48		
ATOM	1147	CE1	TYR	156	44.624	30.889	49.968	1.00	16.29		
ATOM	1148	CD2	TYR	156	43.700	31.012	47.341	1.00	14.47		
ATOM	1149	CE2	TYR	156	44.899	30.288	47.646	1.00	14.32		
ATOM	1150	CZ	TYR	156	45.346	30.240	48.960	1.00	14.29		
ATOM	1151	OH	TYR	156	46.495	29.567	49.289	1.00	12.28		
ATOM	1152	C	TYR	156	40.736	34.600	47.365	1.00	7.25		
ATOM	1153	O	TYR	156	40.152	35.204	48.256	1.00	8.19		
ATOM	1154	N	GLU	157	40.286	34.531	46.107	1.00	4.99		
ATOM	1155	CA	GLU	157	38.979	35.038	45.720	1.00	4.80		
ATOM	1156	CB	GLU	157	39.036	36.256	44.813	1.00	4.31		
ATOM	1157	CG	GLU	157	37.632	36.826	44.614	1.00	3.87		
ATOM	1158	CD	GLU	157	37.577	38.030	43.726	1.00	2.35		
ATOM	1159	OE1	GLU	157	37.568	39.171	44.232	1.00	2.70		
ATOM	1160	OE2	GLU	157	37.486	37.826	42.514	1.00	5.11		
ATOM	1161	C	GLU	157	38.254	33.920	44.997	1.00	6.19		
ATOM	1162	O	GLU	157	38.799	33.290	44.102	1.00	10.44		

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ATOM	1163	N	VAL	158	37.022	33.675	45.406	1.00	5.40	7	
ATOM	1164	CA	VAL	158	36.196	32.627	44.842	1.00	6.15	5	
ATOM	1165	CB	VAL	158	35.459	31.877	45.954	1.00	3.03	5	
ATOM	1166	CG1	VAL	158	34.655	30.759	45.391	1.00	4.03	5	
ATOM	1167	CG2	VAL	158	36.429	31.369	46.962	1.00	3.63	5	
ATOM	1168	C	VAL	158	35.154	33.186	43.878	1.00	9.07	5	
ATOM	1169	O	VAL	158	34.400	34.103	44.208	1.00	10.93	5	
ATOM	1170	N	ASP	159	35.114	32.622	42.681	1.00	10.57	7	
ATOM	1171	CA	ASP	159	34.147	33.012	41.672	1.00	10.09	5	
ATOM	1172	CB	ASP	159	34.828	33.112	40.327	1.00	11.17	5	
ATOM	1173	CG	ASP	159	33.873	33.473	39.256	1.00	13.89	5	
ATOM	1174	OD1	ASP	159	33.863	32.822	38.172	1.00	13.65	5	
ATOM	1175	OD2	ASP	159	33.093	34.407	39.547	1.00	15.65	5	
ATOM	1176	C	ASP	159	32.997	31.985	41.575	1.00	9.91	5	
ATOM	1177	O	ASP	159	33.227	30.761	41.474	1.00	11.09	5	
ATOM	1178	N	VAL	160	31.766	32.485	41.637	1.00	7.83	7	
ATOM	1179	CA	VAL	160	30.582	31.642	41.535	1.00	5.49	5	
ATOM	1180	CB	VAL	160	29.637	31.774	42.755	1.00	3.19	5	
ATOM	1181	CG1	VAL	160	28.512	30.738	42.742	1.00	3.00	5	
ATOM	1182	CG2	VAL	160	30.362	31.602	44.091	1.00	2.00	5	
ATOM	1183	C	VAL	160	29.842	32.132	40.286	1.00	6.19	5	
ATOM	1184	O	VAL	160	29.364	33.280	40.238	1.00	8.22	5	
ATOM	1185	N	SER	161	29.835	31.272	39.300	1.00	7.72	7	
ATOM	1186	CA	SER	161	29.104	31.475	38.046	1.00	8.29	5	
ATOM	1187	CB	SER	161	30.094	31.628	36.891	1.00	10.26	5	
ATOM	1188	OG	SER	161	30.637	32.951	36.934	1.00	13.94	5	
ATOM	1189	C	SER	161	28.161	30.275	37.938	1.00	7.24	5	
ATOM	1190	O	SER	161	28.601	29.117	38.024	1.00	7.94	5	
ATOM	1191	N	ALA	162	26.885	30.605	37.791	1.00	9.16	7	
ATOM	1192	CA	ALA	162	25.793	29.612	37.784	1.00	12.39	5	
ATOM	1193	CB	ALA	162	24.689	30.055	38.736	1.00	15.24	5	
ATOM	1194	C	ALA	162	25.199	29.394	36.379	1.00	14.12	5	
ATOM	1195	O	ALA	162	25.593	30.044	35.406	1.00	13.91	5	
ATOM	1196	N	GLY	163	24.220	28.499	36.369	1.00	15.85	7	
ATOM	1197	CA	GLY	163	23.598	27.913	35.150	1.00	16.65	5	
ATOM	1198	C	GLY	163	22.561	28.761	34.370	1.00	18.26	5	
ATOM	1199	O	GLY	163	21.996	29.729	34.897	1.00	18.80	5	
ATOM	1200	N	ASN	164	22.416	28.231	33.146	1.00	90.00	7	
ATOM	1201	CA	ASN	164	21.568	28.664	31.994	1.00	90.00	5	
ATOM	1202	CB	ASN	164	20.505	27.625	31.685	1.00	90.00	5	
ATOM	1203	CG	ASN	164	19.337	27.730	32.702	1.00	90.00	5	
ATOM	1204	OD1	ASN	164	19.322	27.033	33.726	1.00	90.00	5	
ATOM	1205	ND2	ASN	164	18.334	28.580	32.511	1.00	90.00	7	
ATOM	1206	C	ASN	164	20.728	29.929	32.186	1.00	90.00	5	
ATOM	1207	O	ASN	164	19.665	29.874	32.817	1.00	90.00	5	
ATOM	1208	N	GLY	165	21.227	31.004	31.601	1.00	90.00	7	
ATOM	1209	CA	GLY	165	20.544	32.321	31.514	1.00	90.00	5	
ATOM	1210	C	GLY	165	20.274	33.048	32.859	1.00	90.00	5	
ATOM	1211	O	GLY	165	19.470	33.987	32.927	1.00	90.00	5	
ATOM	1212	N	ALA	166	20.941	32.706	33.967	1.00	90.00	5	
ATOM	1213	CA	ALA	166	20.602	33.406	35.242	1.00	90.00	5	
ATOM	1214	CB	ALA	166	19.550	32.609	36.015	1.00	90.00	5	
ATOM	1215	C	ALA	166	21.795	33.647	36.188	1.00	90.00	5	
ATOM	1216	O	ALA	166	21.646	33.653	37.421	1.00	90.00	5	
ATOM	1217	N	GLY	167	22.964	33.851	35.614	1.00	11.62	7	
ATOM	1218	CA	GLY	167	24.167	34.185	36.400	1.00	13.44	5	
ATOM	1219	C	GLY	167	24.110	35.688	36.704	1.00	15.68	5	
ATOM	1220	O	GLY	167	23.701	36.494	35.863	1.00	15.58	5	
ATOM	1221	N	SER	168	24.504	36.099	37.909	1.00	17.86	7	
ATOM	1222	CA	SER	168	24.434	37.545	38.252	1.00	18.83	5	
ATOM	1223	CB	SER	168	23.543	37.788	39.465	1.00	21.81	5	
ATOM	1224	OG	SER	168	22.556	38.750	39.118	1.00	22.47	5	
ATOM	1225	C	SER	168	25.820	38.200	38.537	1.00	18.61	5	
ATOM	1226	O	SER	168	25.961	39.425	38.506	1.00	18.81	5	
ATOM	1227	N	VAL	169	26.808	37.379	38.789	1.00	18.64	5	
ATOM	1228	CA	VAL	169	28.218	37.762	39.149	1.00	17.78	5	
ATOM	1229	CB	VAL	169	28.719	39.141	38.657	1.00	19.01	5	
ATOM	1230	CG1	VAL	169	30.262	39.261	38.769	1.00	16.57	5	
ATOM	1231	CG2	VAL	169	28.407	39.441	37.197	1.00	18.24	5	
ATOM	1232	C	VAL	169	28.387	37.796	40.666	1.00	17.25	5	
ATOM	1233	O	VAL	169	28.222	38.845	41.313	1.00	15.44	5	
ATOM	1234	N	GLN	170	28.725	36.631	41.201	1.00	15.91	5	
ATOM	1235	CA	GLN	170	28.905	36.475	42.647	1.00	17.12	5	
ATOM	1236	CB	GLN	170	27.928	35.459	43.231	1.00	19.39	5	
ATOM	1237	CG	GLN	170	27.921	35.468	44.766	1.00	24.35	5	
ATOM	1238	CD	GLN	170	28.202	34.091	45.365	1.00	26.34	5	
ATOM	1239	OE1	GLN	170	27.369	33.192	45.247	1.00	27.24	5	
ATOM	1240	NE2	GLN	170	29.335	33.863	46.004	1.00	28.12	5	

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ATOM	1241	C	GLN	170	30.344	36.030	43.047	1.00	14.76	6
ATOM	1242	O	GLN	170	30.735	34.892	42.819	1.00	10.49	5
ATOM	1243	N	ARG	171	31.101	36.932	43.674	1.00	13.88	7
ATOM	1244	CA	ARG	171	32.477	36.643	44.094	1.00	13.53	6
ATOM	1245	CB	ARG	171	33.441	37.718	43.573	1.00	13.16	6
ATOM	1246	CG	ARG	171	33.545	37.814	42.049	1.00	12.56	6
ATOM	1247	CD	ARG	171	34.460	36.758	41.425	1.00	13.31	6
ATOM	1248	NE	ARG	171	34.628	36.922	39.969	1.00	10.48	7
ATOM	1249	CZ	ARG	171	35.274	37.932	39.376	1.00	8.84	5
ATOM	1250	NH1	ARG	171	35.841	38.899	40.105	1.00	4.37	7
ATOM	1251	NH2	ARG	171	35.304	38.000	38.045	1.00	6.87	7
ATOM	1252	C	ARG	171	32.581	36.543	45.630	1.00	15.23	5
ATOM	1253	O	ARG	171	31.706	37.062	46.350	1.00	17.57	3
ATOM	1254	N	VAL	172	33.651	35.916	46.131	1.00	11.99	7
ATOM	1255	CA	VAL	172	33.816	35.727	47.565	1.00	9.19	6
ATOM	1256	CB	VAL	172	33.473	34.260	48.000	1.00	10.74	6
ATOM	1257	CG1	VAL	172	33.300	34.155	49.521	1.00	5.41	6
ATOM	1258	CG2	VAL	172	32.236	33.745	47.262	1.00	11.43	6
ATOM	1259	C	VAL	172	35.216	35.966	48.031	1.00	9.92	6
ATOM	1260	O	VAL	172	36.134	35.398	47.507	1.00	10.28	8
ATOM	1261	N	GLU	173	35.365	36.778	49.062	1.00	14.35	7
ATOM	1262	CA	GLU	173	36.671	37.041	49.657	1.00	14.21	6
ATOM	1263	CB	GLU	173	36.760	38.463	50.218	1.00	17.07	6
ATOM	1264	CG	GLU	173	36.591	39.569	49.173	1.00	21.96	5
ATOM	1265	CD	GLU	173	37.267	40.903	49.573	1.00	25.14	5
ATOM	1266	OE1	GLU	173	37.709	41.647	48.649	1.00	23.21	3
ATOM	1267	OE2	GLU	173	37.359	41.206	50.803	1.00	26.88	3
ATOM	1268	C	GLU	173	26.910	36.016	50.779	1.00	13.64	6
ATOM	1269	O	GLU	173	36.017	35.720	51.592	1.00	13.24	3
ATOM	1270	N	ILE	174	38.087	35.403	50.719	1.00	14.30	7
ATOM	1271	CA	ILE	174	38.557	34.406	51.669	1.00	14.95	6
ATOM	1272	CB	ILE	174	38.915	33.088	50.966	1.00	12.11	6
ATOM	1273	CG2	ILE	174	40.014	32.388	51.689	1.00	13.06	6
ATOM	1274	CG1	ILE	174	37.679	32.182	50.893	1.00	13.75	6
ATOM	1275	CD1	ILE	174	36.625	32.629	49.917	1.00	12.34	6
ATOM	1276	C	ILE	174	39.802	35.051	52.250	1.00	15.60	6
ATOM	1277	O	ILE	174	40.563	35.693	51.532	1.00	17.19	8
ATOM	1278	N	LEU	175	39.982	34.956	53.558	1.00	16.67	7
ATOM	1279	CA	LEU	175	41.138	35.582	54.166	1.00	16.56	6
ATOM	1280	CB	LEU	175	40.838	35.972	55.609	1.00	15.47	6
ATOM	1281	CG	LEU	175	40.467	37.466	55.733	1.00	16.91	6
ATOM	1282	CD1	LEU	175	40.100	38.112	54.394	1.00	14.03	6
ATOM	1283	CD2	LEU	175	39.345	37.623	56.733	1.00	16.66	6
ATOM	1284	C	LEU	175	42.394	34.753	54.031	1.00	16.41	6
ATOM	1285	O	LEU	175	42.322	33.535	53.838	1.00	17.23	8
ATOM	1286	N	GLU	176	43.542	35.431	54.084	1.00	17.18	7
ATOM	1287	CA	GLU	176	44.842	34.765	53.946	1.00	16.66	6
ATOM	1288	CB	GLU	176	46.000	35.733	54.145	1.00	21.33	6
ATOM	1289	CG	GLU	176	45.963	36.472	55.432	1.00	20.62	6
ATOM	1290	CD	GLU	176	46.145	37.925	55.180	1.00	22.84	6
ATOM	1291	OE1	GLU	176	47.330	38.343	55.218	1.00	23.62	8
ATOM	1292	OE2	GLU	176	45.117	38.626	54.911	1.00	23.22	9
ATOM	1293	C	GLU	176	45.068	33.602	54.852	1.00	12.93	6
ATOM	1294	O	GLU	176	44.875	33.686	56.062	1.00	16.37	3
ATOM	1295	N	GLY	177	45.574	32.545	54.259	1.00	9.95	7
ATOM	1296	CA	GLY	177	45.839	31.341	55.001	1.00	8.11	6
ATOM	1297	C	GLY	177	44.736	20.340	54.827	1.00	7.43	6
ATOM	1298	O	GLY	177	44.990	29.169	54.962	1.00	9.00	8
ATOM	1299	N	ARG	178	43.534	30.787	54.493	1.00	7.50	7
ATOM	1300	CA	ARG	178	42.398	29.882	54.316	1.00	8.26	5
ATOM	1301	CB	ARG	178	41.116	30.660	54.477	1.00	10.81	6
ATOM	1302	CG	ARG	178	41.134	31.621	55.616	1.00	14.76	6
ATOM	1303	CD	ARG	178	40.911	30.920	56.950	1.00	20.12	6
ATOM	1304	NE	ARG	178	41.904	31.285	57.960	1.00	24.00	7
ATOM	1305	CZ	ARG	178	42.400	32.509	58.135	1.00	26.21	6
ATOM	1306	NH1	ARG	178	42.004	33.543	57.381	1.00	27.32	7
ATOM	1307	NH2	ARG	178	43.350	32.687	59.043	1.00	26.51	7
ATOM	1308	C	ARG	178	42.375	29.216	52.954	1.00	7.67	6
ATOM	1309	O	ARG	178	42.486	29.881	51.938	1.00	8.54	8
ATOM	1310	N	THR	179	42.205	27.906	52.934	1.00	7.97	7
ATOM	1311	CA	THR	179	42.145	27.157	51.689	1.00	9.51	6
ATOM	1312	CB	THR	179	43.376	26.310	51.542	1.00	9.72	6
ATOM	1313	CG1	THR	179	43.659	25.703	52.818	1.00	12.75	3
ATOM	1314	CG2	THR	179	44.559	27.162	51.073	1.00	6.02	6
ATOM	1315	C	THR	179	40.872	26.265	51.641	1.00	14.19	6
ATOM	1316	O	THR	179	40.892	25.102	51.155	1.00	15.46	3
ATOM	1317	N	GLU	180	39.770	26.831	52.151	1.00	13.36	7
ATOM	1318	CA	GLU	180	38.469	26.188	52.162	1.00	12.94	6

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ATOM	1319	CB	GLU	180	38.329	25.242	53.340	1.00	14.42	5	
ATOM	1320	CG	GLU	180	37.418	24.052	53.048	1.00	18.37	5	
ATOM	1321	CD	GLU	180	37.112	23.255	54.299	1.00	19.86	5	
ATOM	1322	OE1	GLU	180	36.526	23.877	55.216	1.00	21.31	5	
ATOM	1323	OE2	GLU	180	37.473	22.045	54.387	1.00	18.58	5	
ATOM	1324	C	GLU	180	37.442	27.288	52.301	1.00	14.56	5	
ATOM	1325	O	GLU	180	37.742	28.385	52.782	1.00	14.76	5	
ATOM	1326	N	CYS	181	36.209	26.986	51.934	1.00	13.82	7	
ATOM	1327	CA	CYS	181	35.149	27.967	52.034	1.00	12.64	5	
ATOM	1328	CB	CYS	181	35.382	28.990	50.936	1.00	12.66	5	
ATOM	1329	SG	CYS	181	33.911	29.643	50.288	1.00	13.38	15	
ATOM	1330	C	CYS	181	33.766	27.287	51.905	1.00	13.84	5	
ATOM	1331	O	CYS	181	33.606	26.383	51.086	1.00	15.56	8	
ATOM	1332	N	VAL	182	32.790	27.639	52.743	1.00	13.12	7	
ATOM	1333	CA	VAL	182	31.478	26.985	52.613	1.00	11.97	6	
ATOM	1334	CB	VAL	182	31.093	26.072	53.820	1.00	9.54	5	
ATOM	1335	CG1	VAL	182	32.003	26.307	55.003	1.00	10.81	6	
ATOM	1336	CG2	VAL	182	29.669	26.255	54.193	1.00	8.15	5	
ATOM	1337	C	VAL	182	30.353	27.910	52.171	1.00	12.84	6	
ATOM	1338	O	VAL	182	29.930	28.828	52.872	1.00	13.90	2	
ATOM	1339	N	LEU	183	29.954	27.715	50.930	1.00	11.79	7	
ATOM	1340	CA	LEU	183	28.921	28.515	50.338	1.00	12.76	5	
ATOM	1341	CB	LEU	183	29.052	28.500	48.817	1.00	13.26	5	
ATOM	1342	CG	LEU	183	30.193	29.380	48.350	1.00	11.81	5	
ATOM	1343	CD1	LEU	183	30.636	28.956	46.970	1.00	8.24	5	
ATOM	1344	CD2	LEU	183	29.734	30.852	43.398	1.00	13.01	5	
ATOM	1345	C	LEU	183	27.564	28.027	50.778	1.00	14.24	5	
ATOM	1346	O	LEU	183	27.139	26.887	50.514	1.00	15.09	5	
ATOM	1347	N	SER	184	26.897	28.909	51.487	1.00	14.69	7	
ATOM	1348	CA	SER	184	25.583	28.642	51.998	1.00	16.60	6	
ATOM	1349	CB	SER	184	25.558	29.046	53.461	1.00	17.40	6	
ATOM	1350	OG	SER	184	26.601	28.369	54.144	1.00	18.79	8	
ATOM	1351	C	SER	184	24.671	29.537	51.208	1.00	17.61	6	
ATOM	1352	O	SER	184	25.115	30.545	50.679	1.00	18.84	3	
ATOM	1353	N	ASN	185	23.422	29.140	51.048	1.00	18.50	7	
ATOM	1354	CA	ASN	185	22.479	29.998	50.338	1.00	21.04	6	
ATOM	1355	CB	ASN	185	22.463	31.389	51.008	1.00	27.82	6	
ATOM	1356	CG	ASN	185	22.274	31.330	52.546	1.00	33.52	6	
ATOM	1357	OD1	ASN	185	22.899	32.131	53.270	1.00	36.61	8	
ATOM	1358	ND2	ASN	185	21.392	30.414	53.050	1.00	36.25	7	
ATOM	1359	C	ASN	185	22.641	30.149	49.794	1.00	19.48	6	
ATOM	1360	O	ASN	185	22.967	31.228	43.263	1.00	18.46	8	
ATOM	1361	N	LEU	186	22.329	29.062	43.093	1.00	17.53	7	
ATOM	1362	CA	LEU	186	22.384	28.972	46.635	1.00	15.82	5	
ATOM	1363	CB	LEU	186	23.632	28.170	46.201	1.00	14.99	6	
ATOM	1364	CG	LEU	186	25.006	28.318	46.924	1.00	15.24	5	
ATOM	1365	CD1	LEU	186	25.951	27.172	46.540	1.00	13.51	5	
ATOM	1366	CD2	LEU	186	25.689	29.663	46.637	1.00	14.02	5	
ATOM	1367	C	LEU	186	21.069	28.230	46.261	1.00	16.15	5	
ATOM	1368	O	LEU	186	20.449	27.566	47.116	1.00	16.68	8	
ATOM	1369	N	ARG	187	20.611	28.382	45.019	1.00	15.66	7	
ATOM	1370	CA	ARG	187	19.371	27.749	44.576	1.00	14.27	5	
ATOM	1371	CB	ARG	187	18.845	28.415	43.327	1.00	14.63	5	
ATOM	1372	CG	ARG	187	19.153	29.870	43.263	1.00	19.73	5	
ATOM	1373	CD	ARG	187	18.525	30.512	42.054	1.00	23.74	5	
ATOM	1374	NE	ARG	187	19.218	30.197	40.805	1.00	26.90	7	
ATOM	1375	CZ	ARG	187	18.997	29.109	40.060	1.00	23.07	5	
ATOM	1376	NH1	ARG	187	18.110	28.181	40.430	1.00	29.72	7	
ATOM	1377	NH2	ARG	187	19.594	29.001	33.874	1.00	21.36	7	
ATOM	1378	C	ARG	187	19.528	26.264	44.298	1.00	16.07	5	
ATOM	1379	O	ARG	187	20.608	25.788	43.872	1.00	14.20	5	
ATOM	1380	N	GLY	188	18.413	25.557	44.483	1.00	15.94	7	
ATOM	1381	CA	GLY	188	18.369	24.124	44.291	1.00	17.35	5	
ATOM	1382	C	GLY	188	18.304	23.695	42.842	1.00	18.74	5	
ATOM	1383	O	GLY	188	17.760	24.421	42.016	1.00	20.69	5	
ATOM	1384	N	ARG	189	18.822	22.492	42.563	1.00	20.12	7	
ATOM	1385	CA	ARG	189	18.891	21.885	41.239	1.00	20.15	5	
ATOM	1386	CB	ARG	189	17.495	21.501	40.721	1.00	22.54	5	
ATOM	1387	CG	ARG	189	17.450	20.203	39.871	1.00	25.04	6	
ATOM	1388	CD	ARG	189	17.780	20.447	38.380	1.00	25.32	5	
ATOM	1389	NE	ARG	189	18.570	19.373	37.756	1.00	27.40	7	
ATOM	1390	CZ	ARG	189	18.076	18.215	37.299	1.00	29.60	5	
ATOM	1391	NH1	ARG	189	16.766	17.937	37.405	1.00	30.45	7	
ATOM	1392	NH2	ARG	189	18.888	17.342	35.686	1.00	29.39	7	
ATOM	1393	C	ARG	189	19.610	22.773	40.218	1.00	20.12	5	
ATOM	1394	O	ARG	189	19.406	22.605	39.317	1.00	21.60	5	
ATOM	1395	N	THR	190	20.432	23.719	40.693	1.00	13.12	7	
ATOM	1396	CA	THR	190	21.195	24.611	39.812	1.00	17.05	5	

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ATOM	1397	CB	THR	190	21.494	25.944	40.460	1.00	15.30	5
ATOM	1398	OG1	THR	190	20.370	26.366	41.226	1.00	18.33	5
ATOM	1399	CG2	THR	190	21.869	26.984	39.390	1.00	10.48	5
ATOM	1400	C	THR	190	22.576	24.017	39.612	1.00	17.97	5
ATOM	1401	O	THR	190	23.024	23.222	40.428	1.00	17.12	5
ATOM	1402	N	ARG	191	23.262	24.460	38.563	1.00	18.62	7
ATOM	1403	CA	ARG	191	24.621	24.018	38.253	1.00	18.64	5
ATOM	1404	CB	ARG	191	24.783	23.686	35.746	1.00	23.05	5
ATOM	1405	CG	ARG	191	26.243	23.477	35.278	1.00	28.15	5
ATOM	1406	CD	ARG	191	26.802	22.032	35.502	1.00	29.37	5
ATOM	1407	NE	ARG	191	26.824	21.206	35.274	1.00	31.41	7
ATOM	1408	CZ	ARG	191	27.677	21.329	34.236	1.00	30.79	5
ATOM	1409	NH1	ARG	191	28.650	22.261	34.198	1.00	30.54	7
ATOM	1410	NH2	ARG	191	27.562	20.481	33.210	1.00	30.20	7
ATOM	1411	C	ARG	191	25.471	25.213	38.627	1.00	15.56	5
ATOM	1412	O	ARG	191	25.174	26.344	38.233	1.00	14.09	5
ATOM	1413	N	TYR	192	26.495	24.950	39.417	1.00	12.55	7
ATOM	1414	CA	TYR	192	27.380	25.971	39.901	1.00	11.03	5
ATOM	1415	CB	TYR	192	27.283	26.027	41.411	1.00	10.18	5
ATOM	1416	CG	TYR	192	26.063	26.759	41.890	1.00	13.18	5
ATOM	1417	CD1	TYR	192	26.105	28.138	42.101	1.00	14.17	5
ATOM	1418	CE1	TYR	192	24.949	28.867	42.435	1.00	14.60	5
ATOM	1419	CD2	TYR	192	24.837	26.111	42.039	1.00	14.10	5
ATOM	1420	CE2	TYR	192	23.670	26.840	42.371	1.00	15.93	5
ATOM	1421	CZ	TYR	192	23.745	28.217	42.554	1.00	13.34	5
ATOM	1422	OH	TYR	192	22.618	28.972	42.755	1.00	14.24	5
ATOM	1423	C	TYR	192	28.759	25.557	39.508	1.00	12.33	5
ATOM	1424	O	TYR	192	29.134	24.402	39.680	1.00	12.81	5
ATOM	1425	N	THR	193	29.511	26.491	38.954	1.00	10.45	7
ATOM	1426	CA	THR	193	30.875	26.230	38.535	1.00	7.07	5
ATOM	1427	CB	THR	193	31.036	26.551	37.028	1.00	7.66	5
ATOM	1428	OG1	THR	193	30.030	25.849	36.283	1.00	5.74	5
ATOM	1429	CG2	THR	193	32.399	26.130	36.529	1.00	7.11	5
ATOM	1430	C	THR	193	31.688	27.182	39.383	1.00	7.05	5
ATOM	1431	O	THR	193	31.370	28.369	39.425	1.00	7.20	5
ATOM	1432	N	PHE	194	32.685	26.682	40.113	1.00	8.39	7
ATOM	1433	CA	PHE	194	33.487	27.571	40.967	1.00	5.90	5
ATOM	1434	CB	PHE	194	33.421	27.133	42.427	1.00	6.97	5
ATOM	1435	CG	PHE	194	32.030	26.778	42.900	1.00	8.68	5
ATOM	1436	CD1	PHE	194	31.531	25.492	42.723	1.00	5.87	5
ATOM	1437	CD2	PHE	194	31.222	27.735	43.519	1.00	8.15	5
ATOM	1438	CE1	PHE	194	30.273	25.170	43.150	1.00	8.14	5
ATOM	1439	CE2	PHE	194	29.957	27.412	43.946	1.00	5.23	5
ATOM	1440	CZ	PHE	194	29.482	26.129	43.763	1.00	7.24	5
ATOM	1441	C	PHE	194	34.922	27.565	40.524	1.00	5.55	5
ATOM	1442	O	PHE	194	35.367	26.594	39.934	1.00	6.55	5
ATOM	1443	N	ALA	195	35.646	28.633	40.849	1.00	5.34	5
ATOM	1444	CA	ALA	195	37.057	28.785	40.494	1.00	4.57	5
ATOM	1445	CB	ALA	195	37.173	29.298	39.047	1.00	5.31	5
ATOM	1446	C	ALA	195	37.747	29.759	41.467	1.00	3.32	5
ATOM	1447	O	ALA	195	37.101	30.692	41.921	1.00	2.79	5
ATOM	1448	N	VAL	196	39.039	29.539	41.773	1.00	2.76	7
ATOM	1449	CA	VAL	196	39.839	30.398	42.689	1.00	3.78	5
ATOM	1450	CB	VAL	196	40.522	29.609	43.869	1.00	2.00	5
ATOM	1451	CG1	VAL	196	40.237	30.276	45.214	1.00	2.00	5
ATOM	1452	CG2	VAL	196	40.117	28.173	43.869	1.00	4.04	5
ATOM	1453	C	VAL	196	41.000	31.085	41.995	1.00	2.07	5
ATOM	1454	O	VAL	196	41.418	30.661	40.931	1.00	5.97	5
ATOM	1455	N	ARG	197	41.531	32.121	42.629	1.00	2.00	7
ATOM	1456	CA	ARG	197	42.687	32.860	42.129	1.00	2.00	5
ATOM	1457	CB	ARG	197	42.279	33.902	41.069	1.00	2.00	5
ATOM	1458	CG	ARG	197	41.384	35.010	41.574	1.00	2.00	5
ATOM	1459	CD	ARG	197	41.062	36.000	40.504	1.00	2.00	5
ATOM	1460	NE	ARG	197	40.345	37.124	41.073	1.00	3.47	7
ATOM	1461	CZ	ARG	197	40.269	38.323	40.517	1.00	2.00	5
ATOM	1462	NH1	ARG	197	40.846	38.550	39.357	1.00	2.00	7
ATOM	1463	NH2	ARG	197	39.763	39.339	41.193	1.00	4.02	5
ATOM	1464	C	ARG	197	43.374	33.489	43.362	1.00	2.09	5
ATOM	1465	O	ARG	197	42.685	33.926	44.280	1.00	3.19	5
ATOM	1466	N	ALA	198	44.710	33.490	43.399	1.00	2.00	5
ATOM	1467	CA	ALA	198	45.475	33.996	44.550	1.00	2.47	5
ATOM	1468	CB	ALA	198	46.420	32.903	45.072	1.00	2.00	5
ATOM	1469	C	ALA	198	46.241	35.326	44.442	1.00	1.39	5
ATOM	1470	O	ALA	198	46.614	35.772	43.340	1.00	2.18	5
ATOM	1471	N	ARG	199	46.542	35.901	45.612	1.00	3.72	5
ATOM	1472	CA	ARG	199	47.250	37.171	45.694	1.00	3.38	5
ATOM	1473	CB	ARG	199	46.226	38.304	45.572	1.00	2.00	5
ATOM	1474	CG	ARG	199	46.784	39.669	45.270	1.00	6.67	5

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ATOM	1475	CD ARG	199	45.938	40.737	45.915	1.00	9.17
ATOM	1476	NE ARG	199	46.306	42.120	45.579	1.00	13.78
ATOM	1477	CZ ARG	199	46.187	42.662	44.363	1.00	15.94
ATOM	1478	NH1 ARG	199	45.738	41.950	43.329	1.00	18.32
ATOM	1479	NH2 ARG	199	46.417	43.954	44.181	1.00	18.45
ATOM	1480	C ARG	199	48.030	37.321	47.023	1.00	5.53
ATOM	1481	O ARG	199	47.555	36.916	48.058	1.00	8.08
ATOM	1482	N MET	200	49.243	37.864	46.984	1.00	5.53
ATOM	1483	CA MET	200	50.015	38.096	48.197	1.00	4.85
ATOM	1484	CB MET	200	51.484	38.423	47.891	1.00	3.73
ATOM	1485	CG MET	200	52.311	37.271	47.346	1.00	4.67
ATOM	1486	SD MET	200	53.261	36.286	48.538	1.00	9.73
ATOM	1487	CE MET	200	52.284	34.975	48.812	1.00	2.41
ATOM	1488	C MET	200	49.340	39.289	48.874	1.00	7.02
ATOM	1489	O MET	200	49.074	40.314	48.228	1.00	6.42
ATOM	1490	N ALA	201	49.050	39.126	50.167	1.00	7.96
ATOM	1491	CA ALA	201	48.369	40.140	50.962	1.00	10.65
ATOM	1492	CB ALA	201	47.633	39.474	52.117	1.00	4.85
ATOM	1493	C ALA	201	49.261	41.285	51.464	1.00	12.36
ATOM	1494	O ALA	201	50.488	41.204	51.453	1.00	13.02
ATOM	1495	N GLU	202	48.622	42.360	51.901	1.00	15.72
ATOM	1496	CA GLU	202	49.336	43.527	52.421	1.00	19.04
ATOM	1497	CB GLU	202	48.428	44.756	52.276	1.00	23.13
ATOM	1498	CG GLU	202	47.650	44.796	50.914	1.00	28.94
ATOM	1499	CD GLU	202	48.360	45.575	49.757	1.00	31.22
ATOM	1500	OE1 GLU	202	49.466	46.164	49.968	1.00	32.80
ATOM	1501	OE2 GLU	202	47.774	45.613	48.634	1.00	30.41
ATOM	1502	C GLU	202	49.785	43.317	53.903	1.00	19.11
ATOM	1503	O GLU	202	49.394	42.327	54.561	1.00	20.41
ATOM	1504	N PRO	203	50.696	44.173	54.411	1.00	16.25
ATOM	1505	CD PRO	203	51.150	44.143	55.820	1.00	15.32
ATOM	1506	CA PRO	203	51.322	45.290	53.714	1.00	14.26
ATOM	1507	CB PRO	203	51.339	46.367	54.782	1.00	13.02
ATOM	1508	CG PRO	203	51.846	45.538	55.984	1.00	16.38
ATOM	1509	C PRO	203	52.740	44.892	53.356	1.00	12.03
ATOM	1510	O PRO	203	53.537	45.743	52.985	1.00	15.28
ATOM	1511	N SER	204	53.073	43.623	53.540	1.00	8.98
ATOM	1512	CA SER	204	54.420	43.146	53.222	1.00	11.79
ATOM	1513	CB SER	204	54.674	41.764	53.868	1.00	11.87
ATOM	1514	OG SER	204	55.093	41.856	55.224	1.00	12.48
ATOM	1515	C SER	204	54.686	43.060	51.696	1.00	11.88
ATOM	1516	O SER	204	55.632	43.660	51.152	1.00	11.24
ATOM	1517	N PHE	205	53.818	42.309	51.031	1.00	10.89
ATOM	1518	CA PHE	205	53.901	42.074	49.624	1.00	8.76
ATOM	1519	CB PHE	205	53.911	40.573	49.390	1.00	8.70
ATOM	1520	CG PHE	205	55.073	39.862	50.052	1.00	12.81
ATOM	1521	CD1 PHE	205	54.854	38.885	51.029	1.00	11.19
ATOM	1522	CD2 PHE	205	56.388	40.136	49.668	1.00	11.00
ATOM	1523	CE1 PHE	205	55.921	38.198	51.599	1.00	7.35
ATOM	1524	CE2 PHE	205	57.452	39.449	50.237	1.00	11.11
ATOM	1525	CZ PHE	205	57.215	38.480	51.202	1.00	8.98
ATOM	1526	C PHE	205	52.743	42.728	48.900	1.00	8.87
ATOM	1527	O PHE	205	51.756	43.147	49.509	1.00	9.29
ATOM	1528	N GLY	206	52.913	42.864	47.592	1.00	8.57
ATOM	1529	CA GLY	206	51.892	43.459	46.751	1.00	8.14
ATOM	1530	C GLY	206	52.007	42.855	45.367	1.00	7.24
ATOM	1531	O GLY	206	52.956	42.124	45.081	1.00	8.58
ATOM	1532	N GLY	207	51.020	43.080	44.520	1.00	7.18
ATOM	1533	CA GLY	207	51.122	42.534	43.176	1.00	7.59
ATOM	1534	C GLY	207	49.825	42.355	42.430	1.00	4.80
ATOM	1535	O GLY	207	48.857	43.048	42.656	1.00	5.05
ATOM	1536	N PHE	208	49.784	41.332	41.608	1.00	3.71
ATOM	1537	CA PHE	208	48.621	41.069	40.805	1.00	3.73
ATOM	1538	CB PHE	208	49.034	41.071	39.322	1.00	6.46
ATOM	1539	CG PHE	208	50.158	42.013	39.011	1.00	6.53
ATOM	1540	CD1 PHE	208	49.956	43.377	39.004	1.00	6.75
ATOM	1541	CD2 PHE	208	51.441	41.530	38.793	1.00	9.68
ATOM	1542	CE1 PHE	208	51.022	44.253	38.790	1.00	7.99
ATOM	1543	CE2 PHE	208	52.506	42.393	38.579	1.00	8.12
ATOM	1544	CZ PHE	208	52.292	43.756	38.580	1.00	6.95
ATOM	1545	C PHE	208	47.896	39.767	41.149	1.00	2.21
ATOM	1546	O PHE	208	48.463	38.823	41.704	1.00	2.77
ATOM	1547	N TRP	209	46.602	39.780	40.878	1.00	2.30
ATOM	1548	CA TRP	209	45.766	38.625	41.073	1.00	3.71
ATOM	1549	CB TRP	209	44.302	38.979	40.811	1.00	4.79
ATOM	1550	CG TRP	209	43.505	39.373	42.011	1.00	4.76
ATOM	1551	CD2 TRP	209	43.156	38.550	43.104	1.00	2.67
ATOM	1552	CE2 TRP	209	42.347	39.315	43.959	1.00	2.87



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ATOM	1553	CE3	TRP	209	43.445	37.234	43.446	1.00	2.00	6
ATOM	1554	CD1	TRP	209	42.908	40.586	42.240	1.00	2.25	6
ATOM	1555	NE1	TRP	209	42.211	40.554	43.396	1.00	2.00	7
ATOM	1556	C22	TRP	209	41.825	36.809	45.148	1.00	4.70	6
ATOM	1557	C23	TRP	209	42.933	36.729	44.616	1.00	4.57	6
ATOM	1558	CH2	TRP	209	42.131	37.513	45.461	1.00	4.76	6
ATOM	1559	C	TRP	209	46.222	37.604	40.033	1.00	3.17	6
ATOM	1560	O	TRP	209	46.556	37.969	38.920	1.00	3.26	6
ATOM	1561	N	SER	210	46.235	36.335	40.412	1.00	4.99	7
ATOM	1562	CA	SER	210	46.650	35.269	39.533	1.00	5.25	6
ATOM	1563	CB	SER	210	46.903	34.002	40.337	1.00	4.60	6
ATOM	1564	OG	SER	210	45.683	32.363	40.660	1.00	3.40	6
ATOM	1565	C	SER	210	45.571	34.968	38.515	1.00	9.36	6
ATOM	1566	O	SER	210	44.564	35.689	38.398	1.00	13.86	6
ATOM	1567	N	ALA	211	45.832	33.924	37.735	1.00	10.41	7
ATOM	1568	CA	ALA	211	44.895	33.423	36.757	1.00	10.30	6
ATOM	1569	CB	ALA	211	45.639	32.571	35.768	1.00	10.37	6
ATOM	1570	C	ALA	211	43.893	32.558	37.567	1.00	11.25	6
ATOM	1571	O	ALA	211	44.160	32.175	38.706	1.00	14.78	6
ATOM	1572	N	TRP	212	42.736	32.263	37.014	1.00	9.47	7
ATOM	1573	CA	TRP	212	41.791	31.433	37.734	1.00	7.74	6
ATOM	1574	CB	TRP	212	40.447	31.434	36.993	1.00	9.05	6
ATOM	1575	CG	TRP	212	39.723	32.765	36.942	1.00	4.98	6
ATOM	1576	CD2	TRP	212	39.061	33.399	38.030	1.00	2.00	6
ATOM	1577	CE2	TRP	212	38.529	34.597	37.547	1.00	2.33	6
ATOM	1578	CE3	TRP	212	38.867	33.063	39.367	1.00	2.00	6
ATOM	1579	CD1	TRP	212	39.566	33.576	35.867	1.00	2.00	6
ATOM	1580	NE1	TRP	212	38.850	34.680	36.219	1.00	2.00	7
ATOM	1581	C22	TRP	212	37.811	35.470	35.359	1.00	4.55	6
ATOM	1582	C23	TRP	212	38.162	33.921	40.167	1.00	2.47	6
ATOM	1583	CH2	TRP	212	37.640	35.111	39.671	1.00	2.13	6
ATOM	1584	C	TRP	212	42.340	30.012	37.771	1.00	8.93	6
ATOM	1585	O	TRP	212	43.262	29.696	37.043	1.00	8.63	6
ATOM	1586	N	SER	213	41.771	29.145	38.598	1.00	11.16	7
ATOM	1587	CA	SER	213	42.222	27.747	38.642	1.00	11.60	6
ATOM	1588	CB	SER	213	42.041	27.183	40.045	1.00	12.78	6
ATOM	1589	OG	SER	213	40.667	27.131	40.397	1.00	13.18	6
ATOM	1590	C	SER	213	41.303	26.959	37.738	1.00	12.67	6
ATOM	1591	O	SER	213	40.265	27.471	37.293	1.00	14.82	6
ATOM	1592	N	GLU	214	41.644	25.718	37.441	1.00	12.59	7
ATOM	1593	CA	GLU	214	40.694	24.971	35.660	1.00	12.29	6
ATOM	1594	CB	GLU	214	41.307	23.662	36.198	1.00	16.37	6
ATOM	1595	CG	GLU	214	42.107	22.797	34.873	1.00	23.12	6
ATOM	1596	CD	GLU	214	41.249	24.291	33.640	1.00	27.82	6
ATOM	1597	OE1	GLU	214	41.627	25.337	33.001	1.00	29.07	6
ATOM	1598	OE2	GLU	214	40.218	23.631	33.301	1.00	27.91	6
ATOM	1599	C	GLU	214	39.550	24.814	37.680	1.00	11.57	6
ATOM	1600	O	GLU	214	39.793	24.625	38.864	1.00	11.66	6
ATOM	1601	N	PRO	215	38.301	25.037	37.258	1.00	11.02	7
ATOM	1602	CD	PRO	215	37.959	25.363	35.868	1.00	12.93	6
ATOM	1603	CA	PRO	215	37.068	24.965	38.059	1.00	11.49	6
ATOM	1604	CB	PRO	215	36.155	25.896	37.290	1.00	9.49	6
ATOM	1605	CG	PRO	215	36.430	25.447	35.937	1.00	12.12	6
ATOM	1606	C	PRO	215	36.378	23.609	38.237	1.00	9.78	6
ATOM	1607	O	PRO	215	36.664	22.654	37.525	1.00	12.44	6
ATOM	1608	N	VAL	216	35.440	22.553	39.172	1.00	7.47	7
ATOM	1609	CA	VAL	216	34.669	22.346	39.434	1.00	7.05	6
ATOM	1610	CB	VAL	216	34.740	21.829	40.924	1.00	8.24	6
ATOM	1611	CG1	VAL	216	35.569	20.568	41.016	1.00	9.46	6
ATOM	1612	CG2	VAL	216	35.226	22.929	41.918	1.00	6.68	6
ATOM	1613	C	VAL	216	33.261	22.834	39.259	1.00	9.31	6
ATOM	1614	O	VAL	216	33.001	24.039	39.445	1.00	10.20	6
ATOM	1615	N	SER	217	32.357	21.913	38.937	1.00	8.47	7
ATOM	1616	CA	SER	217	30.952	22.247	39.766	1.00	9.61	6
ATOM	1617	CB	SER	217	30.549	22.157	37.302	1.00	10.53	6
ATOM	1618	OG	SER	217	29.610	22.170	37.004	1.00	13.22	6
ATOM	1619	C	SER	217	30.127	21.282	39.601	1.00	10.91	6
ATOM	1620	O	SER	217	30.424	20.961	39.647	1.00	9.60	6
ATOM	1621	N	LEU	218	29.067	21.791	40.224	1.00	10.82	6
ATOM	1622	CA	LEU	218	28.222	20.981	41.102	1.00	11.10	6
ATOM	1623	CB	LEU	218	28.605	21.295	42.566	1.00	9.62	6
ATOM	1624	CG	LEU	218	27.995	20.615	43.789	1.00	6.92	6
ATOM	1625	CD1	LEU	218	28.207	19.153	43.696	1.00	9.37	6
ATOM	1626	CD2	LEU	218	28.647	21.135	45.053	1.00	8.78	6
ATOM	1627	C	LEU	218	26.727	21.208	43.903	1.00	11.91	6
ATOM	1628	O	LEU	218	26.306	22.335	40.693	1.00	12.22	6
ATOM	1629	N	LEU	219	25.958	20.114	40.870	1.00	14.15	6
ATOM	1630	CA	LEU	219	24.486	20.164	40.760	1.00	13.92	6

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ATOM	1631	CB LEU	219	23.867	18.872	40.209	1.00	13.95	5
ATOM	1632	CG LEU	219	23.819	18.429	38.736	1.00	16.57	5
ATOM	1633	CD1 LEU	219	22.857	19.303	37.947	1.00	18.05	5
ATOM	1634	CD2 LEU	219	25.208	18.413	38.096	1.00	15.67	5
ATOM	1635	C LEU	219	24.080	20.226	42.248	1.00	12.96	5
ATOM	1636	O LEU	219	24.378	19.295	42.986	1.00	12.64	5
ATOM	1637	N THR	220	23.501	21.339	42.692	1.00	12.52	7
ATOM	1638	CA THR	220	23.057	21.472	44.068	1.00	10.27	5
ATOM	1639	CB THR	220	22.289	22.744	44.250	1.00	10.53	5
ATOM	1640	OG1 THR	220	22.030	23.333	42.967	1.00	14.44	5
ATOM	1641	CG2 THR	220	23.076	23.764	45.099	1.00	13.55	5
ATOM	1642	C THR	220	22.111	20.325	44.368	1.00	11.61	5
ATOM	1643	O THR	220	21.196	20.053	43.582	1.00	13.03	5
ATOM	1644	N THR	303	67.975	42.354	64.372	1.00	11.41	7
ATOM	1645	CA THR	303	67.750	41.634	65.597	1.00	9.49	5
ATOM	1646	CB THR	303	66.400	42.008	66.344	1.00	10.05	5
ATOM	1647	OG1 THR	303	65.988	43.329	65.963	1.00	12.85	5
ATOM	1648	CG2 THR	303	66.595	42.033	67.861	1.00	12.80	5
ATOM	1649	C THR	303	67.737	40.103	65.280	1.00	9.93	5
ATOM	1650	O THR	303	68.525	39.342	65.838	1.00	9.37	5
ATOM	1651	N TYR	304	66.882	39.690	64.343	1.00	10.17	7
ATOM	1652	CA TYR	304	66.756	38.281	63.973	1.00	8.53	5
ATOM	1653	CB TYR	304	65.306	37.826	64.148	1.00	7.06	5
ATOM	1654	CG TYR	304	64.839	37.937	65.585	1.00	7.97	5
ATOM	1655	CD1 TYR	304	64.311	39.123	66.072	1.00	4.80	5
ATOM	1656	CE1 TYR	304	64.003	39.258	67.389	1.00	3.80	5
ATOM	1657	CD2 TYR	304	65.030	36.883	66.486	1.00	6.93	5
ATOM	1658	CE2 TYR	304	64.721	37.315	67.809	1.00	4.43	5
ATOM	1659	CZ TYR	304	64.208	38.211	68.261	1.00	4.88	5
ATOM	1660	CH TYR	304	63.886	38.359	69.598	1.00	10.24	5
ATOM	1661	C TYR	304	67.182	38.065	62.554	1.00	8.33	5
ATOM	1662	O TYR	304	67.277	39.024	61.804	1.00	11.69	5
ATOM	1663	N SER	305	67.474	36.819	62.201	1.00	9.34	7
ATOM	1664	CA SER	305	67.856	36.442	60.843	1.00	9.43	5
ATOM	1665	CB SER	305	69.204	35.705	60.838	1.00	13.12	5
ATOM	1666	OG SER	305	70.226	36.516	61.427	1.00	18.03	5
ATOM	1667	C SER	305	66.736	35.557	60.273	1.00	10.05	5
ATOM	1668	O SER	305	66.490	34.433	60.754	1.00	10.34	5
ATOM	1669	N CYS	306	66.093	36.051	59.218	1.00	8.05	7
ATOM	1670	CA CYS	306	64.968	35.364	58.619	1.00	5.52	5
ATOM	1671	C CYS	306	64.970	35.039	57.131	1.00	6.70	5
ATOM	1672	O CYS	306	65.609	35.702	56.302	1.00	6.69	5
ATOM	1673	CB CYS	306	63.738	36.188	58.889	1.00	6.36	5
ATOM	1674	SG CYS	306	63.703	36.826	60.556	1.00	8.87	15
ATOM	1675	N HIS	307	64.186	34.026	56.808	1.00	6.09	7
ATOM	1676	CA HIS	307	64.015	33.604	55.459	1.00	7.50	5
ATOM	1677	CB HIS	307	65.038	32.519	55.083	1.00	11.44	5
ATOM	1678	CG HIS	307	64.853	31.183	55.746	1.00	14.32	5
ATOM	1679	CD2 HIS	307	64.068	30.124	55.420	1.00	16.07	5
ATOM	1680	ND1 HIS	307	65.704	30.723	56.734	1.00	16.54	7
ATOM	1681	CE1 HIS	307	65.467	29.448	56.976	1.00	14.82	5
ATOM	1682	NE2 HIS	307	64.478	29.056	56.192	1.00	17.24	7
ATOM	1683	C HIS	307	62.576	33.176	55.236	1.00	9.06	5
ATOM	1684	O HIS	307	61.811	32.393	56.188	1.00	11.93	5
ATOM	1685	N PHE	308	62.167	33.136	53.980	1.00	8.50	7
ATOM	1686	CA PHE	308	60.815	32.725	53.647	1.00	6.53	5
ATOM	1687	CB PHE	308	60.481	32.392	52.187	1.00	7.92	5
ATOM	1688	CG PHE	308	60.530	34.557	51.891	1.00	5.48	5
ATOM	1689	CD1 PHE	308	61.140	35.016	50.747	1.00	6.64	5
ATOM	1690	CD2 PHE	308	59.935	35.482	52.738	1.00	9.42	5
ATOM	1691	CE1 PHE	308	61.152	36.402	50.448	1.00	3.48	5
ATOM	1692	CE2 PHE	308	59.942	36.875	52.445	1.00	3.15	5
ATOM	1693	CD PHE	308	60.547	37.224	51.307	1.00	6.33	5
ATOM	1694	O PHE	308	60.689	31.207	53.849	1.00	5.44	5
ATOM	1695	C PHE	308	61.489	30.424	53.322	1.00	5.17	5
ATOM	1696	N GLY	309	59.746	30.803	54.691	1.00	5.25	7
ATOM	1697	CA GLY	309	59.517	29.331	54.922	1.00	5.83	5
ATOM	1698	C GLY	309	58.215	28.976	54.098	1.00	6.57	5
ATOM	1699	O GLY	309	57.806	29.766	53.316	1.00	8.19	5
ATOM	1700	N PRO	310	57.791	27.766	54.223	1.00	6.60	7
ATOM	1701	CD PRO	310	58.486	26.582	54.742	1.00	3.84	5
ATOM	1702	CA PRO	310	56.646	27.439	53.364	1.00	8.55	5
ATOM	1703	CB PRO	310	56.581	25.937	53.449	1.00	0.33	5
ATOM	1704	CG PRO	310	57.958	25.497	53.857	1.00	10.25	5
ATOM	1705	C PRO	310	55.295	26.077	53.909	1.00	9.53	5
ATOM	1706	O PRO	310	54.387	28.241	53.137	1.00	12.07	5
ATOM	1707	N LEU	311	55.322	28.503	55.161	1.00	9.08	7
ATOM	1708	CA LEU	311	54.145	29.114	55.756	1.00	5.58	5

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ATOM	1709	CB LEU 311	53.834	28.437	57.080	1.00	4.94	
ATOM	1710	CG LEU 311	52.837	27.277	57.127	1.00	5.04	
ATOM	1711	CD1 LEU 311	51.524	27.802	57.619	1.00	5.36	
ATOM	1712	CD2 LEU 311	52.684	26.580	55.781	1.00	5.32	
ATOM	1713	C LEU 311	54.346	30.580	56.002	1.00	4.95	
ATOM	1714	C LEU 311	53.586	31.411	55.540	1.00	4.76	
ATOM	1715	N THR 312	55.390	30.898	56.741	1.00	5.21	
ATOM	1716	CA THR 312	55.680	32.285	57.075	1.00	7.32	
ATOM	1717	CB THR 312	54.772	32.732	58.256	1.00	7.52	
ATOM	1718	CG1 THR 312	54.898	34.144	58.476	1.00	10.56	
ATOM	1719	CG2 THR 312	55.115	31.951	59.526	1.00	6.36	
ATOM	1720	C THR 312	57.168	32.342	57.444	1.00	6.58	
ATOM	1721	O THR 312	57.868	31.352	57.215	1.00	7.15	
ATOM	1722	N TRP 313	57.641	33.477	57.979	1.00	5.96	
ATOM	1723	CA TRP 313	59.050	33.653	58.382	1.00	6.02	
ATOM	1724	CB TRP 313	59.294	35.032	58.992	1.00	2.13	
ATOM	1725	CG TRP 313	58.937	36.213	58.158	1.00	5.28	
ATOM	1726	CD2 TRP 313	59.685	36.779	57.066	1.00	6.34	
ATOM	1727	CE2 TRP 313	59.026	37.968	56.682	1.00	4.38	
ATOM	1728	CE3 TRP 313	60.845	36.403	56.382	1.00	9.66	
ATOM	1729	CD1 TRP 313	57.883	37.044	58.359	1.00	4.69	
ATOM	1730	NE1 TRP 313	57.933	38.103	57.488	1.00	5.00	
ATOM	1731	C22 TRP 313	59.484	38.784	55.656	1.00	4.75	
ATOM	1732	C23 TRP 313	61.301	37.222	55.350	1.00	5.62	
ATOM	1733	CH2 TRP 313	60.618	38.398	55.004	1.00	5.72	
ATOM	1734	C TRP 313	59.605	32.619	59.389	1.00	3.38	
ATOM	1735	C TRP 313	58.931	32.186	60.359	1.00	9.40	
ATOM	1736	N VAL 314	60.847	32.216	59.139	1.00	7.40	
ATOM	1737	CA VAL 314	61.533	31.286	60.013	1.00	8.87	
ATOM	1738	CB VAL 314	62.145	30.110	59.249	1.00	4.82	
ATOM	1739	CG1 VAL 314	62.868	29.204	60.190	1.00	3.24	
ATOM	1740	CG2 VAL 314	61.099	29.333	58.536	1.00	3.95	
ATOM	1741	C VAL 314	62.637	32.192	60.499	1.00	8.62	
ATOM	1742	O VAL 314	63.512	32.562	59.730	1.00	11.03	
ATOM	1743	N CYS 315	62.516	32.672	61.724	1.00	9.61	
ATOM	1744	CA CYS 315	63.524	33.567	62.250	1.00	10.57	
ATOM	1745	C CYS 315	64.417	32.948	63.293	1.00	10.10	
ATOM	1746	C CYS 315	64.191	31.825	63.748	1.00	11.89	
ATOM	1747	CB CYS 315	62.905	34.861	62.757	1.00	10.52	
ATOM	1748	SG CYS 315	62.176	35.824	61.399	1.00	7.84	
ATOM	1749	N LYS 316	65.402	33.724	63.715	1.00	10.83	
ATOM	1750	CA LYS 316	66.381	33.242	64.650	1.00	9.93	
ATOM	1751	CB LYS 316	67.301	32.320	63.860	1.00	10.47	
ATOM	1752	CG LYS 316	68.200	31.444	64.637	1.00	12.32	
ATOM	1753	CD LYS 316	69.242	30.818	63.708	1.00	13.72	
ATOM	1754	CE LYS 316	70.213	31.865	63.178	1.00	17.21	
ATOM	1755	NZ LYS 316	71.029	32.467	64.288	1.00	17.34	
ATOM	1756	C LYS 316	67.141	34.482	65.092	1.00	10.52	
ATOM	1757	O LYS 316	67.192	35.468	64.359	1.00	7.31	
ATOM	1758	N PRO 317	67.592	34.516	65.355	1.00	9.25	
ATOM	1759	CD PRO 317	67.284	33.617	67.471	1.00	7.38	
ATOM	1760	CA PRO 317	68.344	35.662	66.855	1.00	10.51	
ATOM	1761	CB PRO 317	68.365	35.412	68.348	1.00	6.33	
ATOM	1762	CG PRO 317	68.381	33.979	68.426	1.00	6.27	
ATOM	1763	C PRO 317	69.773	35.714	66.285	1.00	14.13	
ATOM	1764	O PRO 317	70.532	34.732	66.339	1.00	14.55	
ATOM	1765	N GLN 318	70.105	36.867	65.711	1.00	16.42	
ATOM	1766	CA GLN 318	71.418	37.137	65.144	1.00	15.93	
ATOM	1767	CB GLN 318	71.369	38.436	64.326	1.00	15.13	
ATOM	1768	CG GLN 318	72.010	38.325	62.946	1.00	15.24	
ATOM	1769	CD GLN 318	71.602	39.482	62.064	1.00	17.19	
ATOM	1770	CE1 GLN 318	70.734	39.341	61.189	1.00	15.60	
ATOM	1771	NE2 GLN 318	72.199	40.642	62.305	1.00	16.42	
ATOM	1772	C GLN 318	72.272	37.385	66.360	1.00	14.25	
ATOM	1773	O GLN 318	71.906	38.227	67.174	1.00	15.24	
ATOM	1774	N THR 403	70.252	35.791	55.614	1.00	11.35	
ATOM	1775	CA THR 403	69.393	36.053	54.455	1.00	12.39	
ATOM	1776	CB THR 403	68.336	34.931	54.252	1.00	15.65	
ATOM	1777	CG1 THR 403	68.911	33.658	54.627	1.00	15.35	
ATOM	1778	CG2 THR 403	57.869	34.823	52.748	1.00	12.39	
ATOM	1779	C THR 403	68.757	37.471	54.551	1.00	11.13	
ATOM	1780	O THR 403	69.149	38.341	53.757	1.00	11.39	
ATOM	1781	N TYR 404	57.778	37.634	55.454	1.00	8.65	
ATOM	1782	CA TYR 404	57.195	39.041	55.682	1.00	6.10	
ATOM	1783	CB TYR 404	65.698	39.115	55.366	1.00	3.26	
ATOM	1784	CG TYR 404	65.323	38.965	53.910	1.00	5.42	
ATOM	1785	CD1 TYR 404	65.036	37.707	52.377	1.00	3.72	
ATOM	1786	CE1 TYR 404	64.723	37.545	52.042	1.00	2.00	

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ATOM	1787	CD2 TYR	404	65.299	40.071	53.050	1.00	2.00
ATOM	1788	CE2 TYR	404	64.992	39.918	51.710	1.00	2.00
ATOM	1789	CZ TYR	404	64.709	38.650	51.219	1.00	2.53
ATOM	1790	OH TYR	404	64.447	38.463	49.891	1.00	6.21
ATOM	1791	C TYR	404	67.374	39.373	57.169	1.00	6.87
ATOM	1792	O TYR	404	67.459	38.477	58.006	1.00	5.71
ATOM	1793	N SER	405	67.453	40.653	57.500	1.00	7.44
ATOM	1794	CA SER	405	67.581	41.068	58.894	1.00	7.96
ATOM	1795	CB SER	405	68.842	41.887	59.094	1.00	9.81
ATOM	1796	OG SER	405	69.985	41.082	59.888	1.00	14.61
ATOM	1797	C SER	405	66.332	41.863	59.305	1.00	10.09
ATOM	1798	O SER	405	66.154	43.047	58.975	1.00	10.03
ATOM	1799	N CYS	406	65.466	41.198	60.046	1.00	10.45
ATOM	1800	CA CYS	406	64.220	41.789	60.452	1.00	10.00
ATOM	1801	C CYS	406	64.192	42.035	61.938	1.00	10.98
ATOM	1802	O CYS	406	64.900	41.386	62.709	1.00	12.25
ATOM	1803	CB CYS	406	63.096	40.827	60.107	1.00	12.32
ATOM	1804	SG CYS	406	63.277	39.951	58.514	1.00	12.21
ATOM	1805	N HIS	407	63.363	42.987	62.332	1.00	10.98
ATOM	1806	CA HIS	407	63.162	43.317	63.721	1.00	8.89
ATOM	1807	CB HIS	407	64.007	44.542	64.165	1.00	11.52
ATOM	1808	CG HIS	407	63.779	45.803	63.370	1.00	12.77
ATOM	1809	CD2 HIS	407	64.324	46.233	62.204	1.00	11.11
ATOM	1810	ND1 HIS	407	62.968	46.832	63.812	1.00	10.97
ATOM	1811	CE1 HIS	407	63.025	47.837	62.954	1.00	10.32
ATOM	1812	NE2 HIS	407	63.840	47.499	61.969	1.00	10.00
ATOM	1813	C HIS	407	61.687	43.614	63.801	1.00	3.26
ATOM	1814	O HIS	407	61.078	43.935	62.789	1.00	10.54
ATOM	1815	N PHE	408	61.099	43.443	64.976	1.00	7.42
ATOM	1816	CA PHE	408	59.690	43.746	65.168	1.00	6.36
ATOM	1817	CB PHE	408	59.281	43.636	66.643	1.00	5.63
ATOM	1818	CG PHE	408	59.441	42.280	67.218	1.00	3.30
ATOM	1819	CD1 PHE	408	59.675	42.125	68.562	1.00	4.11
ATOM	1820	CD2 PHE	408	59.411	41.158	66.409	1.00	4.22
ATOM	1821	CE1 PHE	408	59.888	40.882	69.095	1.00	2.80
ATOM	1822	CE2 PHE	408	59.626	39.885	66.935	1.00	4.80
ATOM	1823	C2 PHE	408	59.866	39.751	68.282	1.00	4.71
ATOM	1824	C PHE	408	59.459	45.185	64.736	1.00	6.02
ATOM	1825	O PHE	408	60.370	46.018	64.744	1.00	8.84
ATOM	1826	N GLY	409	58.231	45.463	64.347	1.00	4.91
ATOM	1827	CA GLY	409	57.868	46.791	63.936	1.00	2.33
ATOM	1828	C GLY	409	56.494	46.954	64.509	1.00	2.02
ATOM	1829	O GLY	409	55.996	46.065	65.196	1.00	4.33
ATOM	1830	N PRO	410	55.879	48.100	64.299	1.00	2.00
ATOM	1831	CD PRO	410	56.497	49.286	63.693	1.00	2.98
ATOM	1832	CA PRO	410	54.544	48.397	64.788	1.00	3.72
ATOM	1833	CB PRO	410	54.276	49.754	64.166	1.00	4.67
ATOM	1834	CG PRO	410	55.623	50.390	64.195	1.00	6.29
ATOM	1835	C PRO	410	53.525	47.367	64.313	1.00	7.04
ATOM	1836	O PRO	410	52.831	46.752	65.137	1.00	8.58
ATOM	1837	N LEU	411	53.471	47.165	62.987	1.00	6.97
ATOM	1838	CA LEU	411	52.544	46.233	62.329	1.00	5.66
ATOM	1839	CB LEU	411	52.254	46.674	60.898	1.00	8.28
ATOM	1840	CG LEU	411	51.310	47.803	60.553	1.00	11.17
ATOM	1841	CD1 LEU	411	50.007	47.519	61.244	1.00	15.07
ATOM	1842	CD2 LEU	411	51.888	49.156	60.961	1.00	14.05
ATOM	1843	C LEU	411	53.052	44.831	62.192	1.00	4.04
ATOM	1844	O LEU	411	52.365	43.870	62.481	1.00	2.78
ATOM	1845	N THR	412	54.237	44.705	61.643	1.00	3.16
ATOM	1846	CA THR	412	54.749	43.388	61.431	1.00	2.09
ATOM	1847	CB THR	412	53.985	42.829	60.244	1.00	2.00
ATOM	1848	CG1 THR	412	54.152	41.413	60.166	1.00	4.84
ATOM	1849	CG2 THR	412	54.417	43.523	58.976	1.00	2.00
ATOM	1850	C THR	412	56.252	43.565	61.220	1.00	2.54
ATOM	1851	O THR	412	56.722	44.675	61.376	1.00	3.52
ATOM	1852	N TRP	413	57.003	42.490	60.964	1.00	3.38
ATOM	1853	CA TRP	413	58.468	42.579	60.747	1.00	4.26
ATOM	1854	CB TRP	413	59.002	41.293	60.115	1.00	3.65
ATOM	1855	CG TRP	413	58.912	40.078	60.909	1.00	2.26
ATOM	1856	CE2 TRP	413	59.722	39.734	62.023	1.00	4.36
ATOM	1857	CE3 TRP	413	59.374	38.418	62.398	1.00	3.95
ATOM	1858	CE1 TRP	413	60.712	40.409	62.745	1.00	5.87
ATOM	1859	NE1 TRP	413	58.121	39.011	60.667	1.00	2.00
ATOM	1860	CD1 TRP	413	58.395	37.998	61.546	1.00	3.14
ATOM	1861	CD2 TRP	413	59.975	37.766	63.459	1.00	7.15
ATOM	1862	C2 TRP	413	61.212	39.764	63.801	1.00	7.66
ATOM	1863	CH2 TRP	413	60.941	38.451	64.152	1.00	8.17
ATOM	1864	C TRP	413	58.960	43.720	59.832	1.00	5.50

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ATOM	1865	I	TRF	413	58.187	44.350	59.115	1.00	7.06	3	
ATOM	1866	N	VAL	414	60.273	43.923	59.813	1.00	6.50	7	
ATOM	1867	CA	VAL	414	60.904	44.921	58.957	1.00	6.63	4	
ATOM	1868	CB	VAL	414	61.076	46.289	59.660	1.00	7.88	3	
ATOM	1869	CG1	VAL	414	62.193	47.072	59.029	1.00	6.76	4	
ATOM	1870	CG2	VAL	414	59.789	47.111	59.547	1.00	3.37	4	
ATOM	1871	C	VAL	414	62.242	44.340	58.533	1.00	9.59	4	
ATOM	1872	I	VAL	414	63.183	44.296	59.303	1.00	11.73	3	
ATOM	1873	N	CYS	415	62.296	43.820	57.314	1.00	9.75	7	
ATOM	1874	CA	CYS	415	63.515	43.222	56.809	1.00	9.19	6	
ATOM	1875	C	CYS	415	64.238	44.007	55.767	1.00	9.05	4	
ATOM	1876	C	CYS	415	63.714	44.949	55.189	1.00	8.76	3	
ATOM	1877	CB	CYS	415	63.207	41.882	56.222	1.00	9.11	4	
ATOM	1878	SG	CYS	415	62.067	41.071	57.341	1.00	14.13	14	
ATOM	1879	N	LYS	416	65.484	43.622	55.581	1.00	7.88	7	
ATOM	1880	CA	LYS	416	66.341	44.197	54.585	1.00	9.50	6	
ATOM	1881	CB	LYS	416	67.176	45.349	55.135	1.00	14.71	6	
ATOM	1882	CG	LYS	416	66.482	46.235	56.144	1.00	19.54	5	
ATOM	1883	CD	LYS	416	66.618	45.629	57.541	1.00	23.24	6	
ATOM	1884	CE	LYS	416	65.851	46.404	58.599	1.00	23.74	6	
ATOM	1885	NZ	LYS	416	66.292	45.888	59.937	1.00	27.08	7	
ATOM	1886	C	LYS	416	67.234	43.008	54.278	1.00	12.10	6	
ATOM	1887	C	LYS	416	67.523	42.187	55.175	1.00	10.95	3	
ATOM	1888	N	PRO	417	67.578	42.817	52.990	1.00	12.45	7	
ATOM	1889	CD	PRO	417	67.231	43.561	51.771	1.00	11.38	6	
ATOM	1890	CA	PRO	417	66.434	41.684	52.671	1.00	11.76	4	
ATOM	1891	CB	PRO	417	68.394	41.647	51.144	1.00	10.58	3	
ATOM	1892	CG	PRO	417	68.247	43.047	50.780	1.00	11.41	3	
ATOM	1893	C	PRO	417	69.845	41.868	53.221	1.00	14.43	3	
ATOM	1894	C	PRO	417	70.361	42.990	53.325	1.00	14.95	3	
ATOM	1895	N	GLN	418	70.400	40.762	53.700	1.00	15.69	7	
ATOM	1896	CA	GLN	418	71.753	40.741	54.209	1.00	16.01	6	
ATOM	1897	CB	GLN	418	71.932	39.562	55.165	1.00	15.85	4	
ATOM	1898	CG	GLN	418	71.948	39.963	56.620	1.00	13.51	6	
ATOM	1899	CD	GLN	418	71.580	38.823	57.530	1.00	16.21	6	
ATOM	1900	OE1	GLN	418	71.377	37.668	57.098	1.00	16.54	3	
ATOM	1901	NE2	GLN	418	71.478	39.131	58.807	1.00	16.18	7	
ATOM	1902	C	GLN	418	72.660	40.583	52.990	1.00	17.91	6	
ATOM	1903	C	GLN	418	72.470	39.656	52.172	1.00	20.26	3	
ATOM	1904	N	LYS	510	36.636	45.747	96.455	1.00	20.08	7	
ATOM	1905	CA	LYS	510	36.983	44.827	97.554	1.00	22.39	4	
ATOM	1906	CB	LYS	510	37.004	45.503	98.958	1.00	22.50	4	
ATOM	1907	CG	LYS	510	37.794	44.729	100.099	1.00	24.41	3	
ATOM	1908	CD	LYS	510	39.382	44.786	99.984	1.00	24.23	3	
ATOM	1909	CE	LYS	510	40.149	44.388	101.309	1.00	25.09	3	
ATOM	1910	NZ	LYS	510	40.281	42.907	101.710	1.00	21.46	3	
ATOM	1911	C	LYS	510	36.039	43.642	97.542	1.00	21.11	4	
ATOM	1912	C	LYS	510	26.117	42.777	98.413	1.00	20.71	3	
ATOM	1913	N	PHE	511	35.089	43.650	96.604	1.00	20.62	4	
ATOM	1914	CA	PHE	511	34.207	42.501	96.453	1.00	18.81	3	
ATOM	1915	CB	PHE	511	32.903	42.833	95.720	1.00	17.03	3	
ATOM	1916	CG	PHE	511	31.969	41.646	95.592	1.00	17.36	3	
ATOM	1917	CD1	PHE	511	32.470	40.353	95.362	1.00	17.10	3	
ATOM	1918	CD2	PHE	511	30.594	41.806	95.735	1.00	19.23	3	
ATOM	1919	CE1	PHE	511	31.630	39.235	95.279	1.00	16.04	3	
ATOM	1920	CE2	PHE	511	29.738	40.690	95.653	1.00	20.47	3	
ATOM	1921	CZ	PHE	511	30.271	39.394	95.424	1.00	17.16	3	
ATOM	1922	C	PHE	511	35.064	41.629	95.554	1.00	17.52	3	
ATOM	1923	I	PHE	511	35.406	40.483	95.913	1.00	16.93	3	
ATOM	1924	N	GLU	512	35.416	42.200	94.392	1.00	17.14	3	
ATOM	1925	CA	GLU	512	36.244	41.509	93.406	1.00	18.20	3	
ATOM	1926	CB	GLU	512	36.536	42.391	92.172	1.00	20.73	3	
ATOM	1927	CG	GLU	512	37.498	41.754	91.075	1.00	28.00	3	
ATOM	1928	CD	GLU	512	36.651	40.687	90.101	1.00	20.11	3	
ATOM	1929	CE1	GLU	512	37.346	40.507	93.936	1.00	29.86	3	
ATOM	1930	CE2	GLU	512	35.865	40.011	90.501	1.00	30.27	3	
ATOM	1931	C	GLU	512	37.507	41.181	94.162	1.00	15.96	3	
ATOM	1932	I	GLU	512	37.938	40.020	94.161	1.00	16.76	3	
ATOM	1933	N	SER	513	37.984	42.163	94.930	1.00	13.17	3	
ATOM	1934	CA	SER	513	39.184	42.008	95.745	1.00	12.13	3	
ATOM	1935	CB	SER	513	39.534	43.314	96.443	1.00	12.70	3	
ATOM	1936	CG	SER	513	40.319	43.054	97.594	1.00	13.07	3	
ATOM	1937	C	SER	513	39.122	40.871	95.775	1.00	12.57	3	
ATOM	1938	I	SER	513	40.041	40.022	95.846	1.00	14.35	3	
ATOM	1939	N	LYS	514	38.056	40.844	97.573	1.00	11.94	7	
ATOM	1940	CA	LYS	514	37.903	39.792	98.568	1.00	9.95	3	
ATOM	1941	CB	LYS	514	36.839	40.121	99.605	1.00	7.59	3	
ATOM	1942	CG	LYS	514	37.256	41.165	100.627	1.00	3.11	3	

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ATOM	1943	CD LYS	514	36.388	41.093	101.842	1.00	2.50
ATOM	1944	CE LYS	514	36.374	42.393	102.539	1.00	2.00
ATOM	1945	NZ LYS	514	35.665	42.215	103.798	1.00	3.28
ATOM	1946	C LYS	514	37.621	36.443	97.959	1.00	11.50
ATOM	1947	O LYS	514	37.841	37.435	98.620	1.00	13.26
ATOM	1948	N ALA	515	37.138	36.401	96.716	1.00	10.50
ATOM	1949	CA ALA	515	36.876	37.117	96.038	1.00	9.26
ATOM	1950	CB ALA	515	36.187	37.366	94.719	1.00	10.99
ATOM	1951	C ALA	515	38.165	36.299	95.806	1.00	8.83
ATOM	1952	O ALA	515	38.170	35.068	95.920	1.00	7.78
ATOM	1953	N ALA	516	39.241	37.026	95.494	1.00	8.76
ATOM	1954	CA ALA	516	40.562	36.478	95.204	1.00	7.65
ATOM	1955	CB ALA	516	41.457	37.533	94.614	1.00	6.46
ATOM	1956	C ALA	516	41.205	35.872	96.419	1.00	7.97
ATOM	1957	O ALA	516	41.690	34.751	96.353	1.00	8.85
ATOM	1958	N LEU	517	41.226	36.599	97.530	1.00	8.04
ATOM	1959	CA LEU	517	41.809	36.040	98.743	1.00	5.52
ATOM	1960	CB LEU	517	41.445	36.874	99.947	1.00	3.15
ATOM	1961	CG LEU	517	42.141	38.193	100.158	1.00	4.53
ATOM	1962	CD1 LEU	517	41.717	39.177	99.108	1.00	8.66
ATOM	1963	CD2 LEU	517	41.754	38.683	101.519	1.00	4.29
ATOM	1964	C LEU	517	41.271	34.634	98.992	1.00	7.39
ATOM	1965	O LEU	517	42.009	33.751	99.437	1.00	10.93
ATOM	1966	N LEU	518	39.997	34.433	93.648	1.00	8.49
ATOM	1967	CA LEU	518	39.297	33.177	98.857	1.00	7.25
ATOM	1968	CB LEU	518	37.845	33.467	99.273	1.00	5.35
ATOM	1969	CG LEU	518	37.614	33.731	100.772	1.00	5.58
ATOM	1970	CD1 LEU	518	36.802	34.965	100.936	1.00	3.48
ATOM	1971	CD2 LEU	518	36.951	32.519	101.495	1.00	6.87
ATOM	1972	C LEU	518	39.339	32.158	97.723	1.00	9.11
ATOM	1973	O LEU	518	39.185	30.955	97.979	1.00	8.10
ATOM	1974	N ALA	519	39.557	32.623	96.505	1.00	11.23
ATOM	1975	CA ALA	519	39.603	31.726	95.342	1.00	13.55
ATOM	1976	CB ALA	519	39.310	32.481	94.072	1.00	12.74
ATOM	1977	C ALA	519	40.908	30.949	95.209	1.00	15.14
ATOM	1978	O ALA	519	41.733	31.215	94.311	1.00	15.55
ATOM	1979	N ALA	520	41.047	29.935	96.068	1.00	17.93
ATOM	1980	CA ALA	520	42.228	29.064	96.115	1.00	19.81
ATOM	1981	CB ALA	520	42.169	28.165	97.371	1.00	20.83
ATOM	1982	C ALA	520	42.579	28.212	94.865	1.00	19.53
ATOM	1983	O ALA	520	41.764	27.430	94.339	1.00	19.39
ATOM	1984	N ARG	521	43.834	28.352	94.449	1.00	90.00
ATOM	1985	CA ARG	521	44.407	27.633	93.322	1.00	90.00
ATOM	1986	CB ARG	521	45.499	28.484	92.652	1.00	90.00
ATOM	1987	CG ARG	521	45.117	29.950	92.441	1.00	90.00
ATOM	1988	CD ARG	521	45.751	30.871	93.500	1.00	90.00
ATOM	1989	NE ARG	521	45.512	30.373	94.854	1.00	90.00
ATOM	1990	CZ ARG	521	46.279	29.452	95.464	1.00	90.00
ATOM	1991	NH1 ARG	521	47.351	28.957	94.843	1.00	90.00
ATOM	1992	NH2 ARG	521	45.886	28.889	96.620	1.00	90.00
ATOM	1993	C ARG	521	45.018	26.343	93.866	1.00	90.00
ATOM	1994	O ARG	521	44.842	26.022	95.032	1.00	90.00
ATOM	1995	N GLY	522	45.710	25.592	93.022	1.00	90.00
ATOM	1996	CA GLY	522	46.338	24.375	93.500	1.00	90.00
ATOM	1997	C GLY	522	47.851	24.578	93.549	1.00	90.00
ATOM	1998	O GLY	522	48.288	25.677	93.891	1.00	90.00
ATOM	1999	N PRO	523	48.672	23.533	93.225	1.00	90.00
ATOM	2000	CD PRO	523	48.070	22.203	92.929	1.00	90.00
ATOM	2001	CA PRO	523	50.157	23.469	93.185	1.00	90.00
ATOM	2002	CB PRO	523	50.429	22.304	92.201	1.00	90.00
ATOM	2003	CG PRO	523	49.277	21.315	92.486	1.00	90.00
ATOM	2004	C PRO	523	50.966	24.731	92.741	1.00	90.00
ATOM	2005	O PRO	523	50.499	25.617	91.984	1.00	90.00
ATOM	2006	N GLU	524	52.222	24.761	93.180	1.00	24.71
ATOM	2007	CA GLU	524	53.121	25.851	92.829	1.00	23.43
ATOM	2008	CB GLU	524	54.289	25.979	93.857	1.00	27.47
ATOM	2009	CG GLU	524	55.487	24.958	93.730	1.00	29.39
ATOM	2010	CD GLU	524	55.207	23.507	94.250	1.00	31.55
ATOM	2011	OE1 GLU	524	54.910	22.603	93.413	1.00	29.10
ATOM	2012	OE2 GLU	524	55.343	23.263	93.484	1.00	30.26
ATOM	2013	C GLU	524	53.672	25.532	91.428	1.00	21.32
ATOM	2014	O GLU	524	53.705	24.359	91.016	1.00	20.22
ATOM	2015	N GLU	525	54.169	26.564	90.747	1.00	18.90
ATOM	2016	CA GLU	525	54.722	26.411	89.427	1.00	18.58
ATOM	2017	CB GLU	525	53.557	26.334	88.442	1.00	18.50
ATOM	2018	CG GLU	525	53.857	25.543	87.149	1.00	27.12
ATOM	2019	CD GLU	525	52.595	25.167	86.357	1.00	31.94
ATOM	2020	OE1 GLU	525	52.474	23.956	85.991	1.00	31.25

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ATOM	2021	OE2 GLU	525	51.731	26.066	85.119	1.00	34.53
ATOM	2022	C GLU	525	55.572	27.633	89.150	1.00	8.91
ATOM	2023	C GLU	525	55.306	28.676	89.733	1.00	9.70
ATOM	2024	N LEU	526	56.619	27.495	88.331	1.00	5.52
ATOM	2025	CA LEU	526	57.455	28.638	87.940	1.00	4.14
ATOM	2026	CB LEU	526	58.859	28.182	87.485	1.00	4.80
ATOM	2027	CG LEU	526	60.103	29.082	87.590	1.00	2.00
ATOM	2028	CD1 LEU	526	61.166	28.507	86.706	1.00	2.00
ATOM	2029	CD2 LEU	526	59.856	30.499	87.193	1.00	2.00
ATOM	2030	C LEU	526	56.688	29.248	86.751	1.00	2.64
ATOM	2031	O LEU	526	56.527	28.607	85.733	1.00	2.80
ATOM	2032	N LEU	527	56.209	30.474	86.892	1.00	2.00
ATOM	2033	CA LEU	527	55.415	31.107	85.854	1.00	2.00
ATOM	2034	CB LEU	527	54.115	31.638	86.441	1.00	4.05
ATOM	2035	CG LEU	527	53.035	30.653	86.824	1.00	2.65
ATOM	2036	CD1 LEU	527	51.951	31.429	87.441	1.00	2.00
ATOM	2037	CD2 LEU	527	52.547	29.889	85.620	1.00	2.00
ATOM	2038	C LEU	527	56.110	32.256	85.176	1.00	4.04
ATOM	2039	O LEU	527	56.413	33.252	85.836	1.00	5.30
ATOM	2040	N CYS	528	56.234	32.176	83.844	1.00	3.62
ATOM	2041	CA CYS	528	56.929	33.199	83.051	1.00	2.97
ATOM	2042	C CYS	528	55.987	33.810	82.044	1.00	2.18
ATOM	2043	O CYS	528	55.087	33.127	81.560	1.00	2.61
ATOM	2044	CB CYS	528	58.132	32.593	82.282	1.00	2.00
ATOM	2045	SG CYS	528	59.491	31.832	83.234	1.00	2.00
ATOM	2046	N PHE	529	56.197	35.088	81.743	1.00	2.00
ATOM	2047	CA PHE	529	55.397	35.792	80.758	1.00	4.16
ATOM	2048	CB PHE	529	54.008	36.143	81.303	1.00	3.88
ATOM	2049	CG PHE	529	53.980	37.315	82.231	1.00	2.00
ATOM	2050	CD1 PHE	529	53.958	38.611	81.733	1.00	2.00
ATOM	2051	CD2 PHE	529	53.912	37.123	83.611	1.00	2.00
ATOM	2052	CE1 PHE	529	53.868	39.697	82.590	1.00	2.00
ATOM	2053	CE2 PHE	529	53.822	38.207	84.471	1.00	2.00
ATOM	2054	CZ PHE	529	53.801	39.490	83.961	1.00	2.00
ATOM	2055	C PHE	529	56.100	37.031	80.200	1.00	5.77
ATOM	2056	O PHE	529	57.078	37.511	80.785	1.00	6.52
ATOM	2057	N THR	530	55.665	37.471	79.018	1.00	2.84
ATOM	2058	CA THR	530	56.225	38.655	78.377	1.00	2.00
ATOM	2059	CB THR	530	57.228	38.280	77.232	1.00	2.00
ATOM	2060	OG1 THR	530	57.683	39.460	76.579	1.00	2.84
ATOM	2061	CG2 THR	530	56.637	37.355	76.234	1.00	2.96
ATOM	2062	C THR	530	55.076	39.582	77.948	1.00	2.59
ATOM	2063	O THR	530	53.999	39.124	77.611	1.00	4.21
ATOM	2064	N GLU	531	55.275	40.882	78.076	1.00	2.29
ATOM	2065	CA GLU	531	54.246	41.854	77.747	1.00	5.46
ATOM	2066	CB GLU	531	54.178	42.919	78.836	1.00	10.50
ATOM	2067	CG GLU	531	54.046	42.346	80.257	1.00	12.93
ATOM	2068	CD GLU	531	53.771	43.413	81.298	1.00	14.12
ATOM	2069	OE1 GLU	531	54.085	44.606	81.079	1.00	15.54
ATOM	2070	OE2 GLU	531	53.227	43.052	82.355	1.00	18.13
ATOM	2071	C GLU	531	54.462	42.489	76.382	1.00	6.42
ATOM	2072	O GLU	531	53.505	42.685	75.650	1.00	9.10
ATOM	2073	N ARG	532	55.659	43.021	76.152	1.00	5.91
ATOM	2074	CA ARG	532	56.039	43.529	74.832	1.00	6.83
ATOM	2075	CB ARG	532	56.900	44.795	74.890	1.00	6.46
ATOM	2076	CG ARG	532	56.141	46.059	75.094	1.00	4.16
ATOM	2077	CD ARG	532	55.682	46.070	76.483	1.00	6.94
ATOM	2078	NE ARG	532	54.531	46.930	76.696	1.00	14.70
ATOM	2079	CZ ARG	532	54.158	47.395	77.890	1.00	17.72
ATOM	2080	NH1 ARG	532	54.877	47.096	78.975	1.00	13.74
ATOM	2081	NH2 ARG	532	52.998	48.056	78.017	1.00	18.08
ATOM	2082	C ARG	532	56.934	42.364	74.424	1.00	3.68
ATOM	2083	O ARG	532	56.904	41.310	73.052	1.00	12.29
ATOM	2084	N LEU	533	57.767	42.502	73.436	1.00	10.64
ATOM	2085	CA LEU	533	58.606	41.256	73.125	1.00	12.12
ATOM	2086	CB LEU	533	58.326	40.790	71.821	1.00	13.13
ATOM	2087	CG LEU	533	56.884	40.298	71.741	1.00	10.95
ATOM	2088	CD1 LEU	533	56.531	39.773	70.348	1.00	11.69
ATOM	2089	CD2 LEU	533	56.773	39.204	72.754	1.00	12.40
ATOM	2090	C LEU	533	60.064	41.733	73.430	1.00	11.88
ATOM	2091	O LEU	533	60.897	41.490	72.535	1.00	12.70
ATOM	2092	N GLU	534	60.365	42.115	74.666	1.00	12.95
ATOM	2093	CA GLU	534	61.722	42.523	75.003	1.00	13.80
ATOM	2094	CB GLU	534	61.999	43.882	74.365	1.00	16.94
ATOM	2095	CG GLU	534	61.006	44.974	74.791	1.00	23.38
ATOM	2096	CD GLU	534	60.768	46.010	73.684	1.00	26.01
ATOM	2097	OE1 GLU	534	59.849	46.860	73.862	1.00	26.36
ATOM	2098	OE2 GLU	534	61.461	45.938	72.625	1.00	25.83

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ATOM	2099	C	GLU	534	61.892	42.579	75.527	1.00 10.95
ATOM	2100	C	GLU	534	62.651	42.380	77.066	1.00 10.92
ATOM	2101	N	ASP	535	61.251	41.637	77.194	1.00 9.01
ATOM	2102	CA	ASP	535	61.247	41.578	78.638	1.00 6.92
ATOM	2103	CB	ASP	535	60.188	42.544	79.128	1.00 8.31
ATOM	2104	CG	ASP	535	58.848	42.334	78.430	1.00 8.75
ATOM	2105	OD1	ASP	535	58.020	41.541	78.913	1.00 11.89
ATOM	2106	OD2	ASP	535	58.635	42.949	77.372	1.00 15.77
ATOM	2107	C	ASP	535	60.793	40.201	79.033	1.00 6.27
ATOM	2108	O	ASP	535	60.062	39.577	78.295	1.00 6.65
ATOM	2109	N	LEU	536	61.176	39.731	80.204	1.00 5.28
ATOM	2110	CA	LEU	536	60.717	38.436	80.651	1.00 4.48
ATOM	2111	CB	LEU	536	61.614	37.315	80.149	1.00 2.00
ATOM	2112	CG	LEU	536	61.012	35.958	80.495	1.00 2.00
ATOM	2113	CD1	LEU	536	59.697	35.789	79.782	1.00 2.00
ATOM	2114	CD2	LEU	536	61.955	34.853	80.152	1.00 2.00
ATOM	2115	C	LEU	536	60.725	38.468	82.154	1.00 5.42
ATOM	2116	O	LEU	536	61.701	38.896	82.751	1.00 5.81
ATOM	2117	N	VAL	537	59.606	38.093	82.767	1.00 6.59
ATOM	2118	CA	VAL	537	59.514	38.050	84.219	1.00 4.71
ATOM	2119	CB	VAL	537	58.439	39.006	84.761	1.00 3.90
ATOM	2120	CG1	VAL	537	58.391	38.900	86.262	1.00 7.66
ATOM	2121	CG2	VAL	537	58.754	40.434	84.386	1.00 6.66
ATOM	2122	C	VAL	537	59.111	36.652	84.604	1.00 2.70
ATOM	2123	O	VAL	537	58.232	36.096	83.977	1.00 5.62
ATOM	2124	N	CYS	538	59.812	36.048	85.553	1.00 3.31
ATOM	2125	CA	CYS	538	59.452	34.711	85.055	1.00 4.73
ATOM	2126	C	CYS	538	59.375	34.771	87.597	1.00 5.86
ATOM	2127	O	CYS	538	60.165	35.457	83.257	1.00 6.30
ATOM	2128	CB	CYS	538	60.438	33.619	85.600	1.00 2.00
ATOM	2129	SC	CYS	538	60.634	33.421	83.795	1.00 3.79
ATOM	2130	N	PHE	539	58.426	34.059	88.178	1.00 3.78
ATOM	2131	CA	PHE	539	58.267	34.099	89.621	1.00 4.15
ATOM	2132	CB	PHE	539	57.295	35.232	89.997	1.00 4.88
ATOM	2133	CG	PHE	539	55.852	35.009	89.515	1.00 7.86
ATOM	2134	CD1	PHE	539	54.835	34.690	90.420	1.00 5.60
ATOM	2135	CD2	PHE	539	55.519	35.104	88.147	1.00 9.65
ATOM	2136	CE1	PHE	539	53.540	34.470	89.986	1.00 4.81
ATOM	2137	CE2	PHE	539	54.201	34.878	87.706	1.00 7.22
ATOM	2138	CZ	PHE	539	53.223	34.562	88.630	1.00 5.52
ATOM	2139	C	PHE	539	57.689	32.807	90.123	1.00 3.30
ATOM	2140	O	PHE	539	57.397	31.913	89.352	1.00 5.07
ATOM	2141	N	TRP	540	57.606	32.696	91.436	1.00 2.62
ATOM	2142	CA	TRP	540	56.965	31.575	92.102	1.00 5.41
ATOM	2143	CB	TRP	540	57.859	30.331	92.252	1.00 5.13
ATOM	2144	CG	TRP	540	58.890	30.380	93.315	1.00 7.06
ATOM	2145	CD2	TRP	540	60.250	30.807	93.175	1.00 4.64
ATOM	2146	CE2	TRP	540	60.861	30.657	94.430	1.00 5.73
ATOM	2147	CE3	TRP	540	61.006	31.299	92.110	1.00 5.86
ATOM	2148	CD1	TRP	540	58.738	29.995	91.610	1.00 8.29
ATOM	2149	NE1	TRP	540	59.914	30.161	95.286	1.00 8.36
ATOM	2150	CZ2	TRP	540	62.208	30.984	94.657	1.00 8.15
ATOM	2151	CZ3	TRP	540	62.336	31.623	92.328	1.00 7.58
ATOM	2152	CH2	TRP	540	62.927	31.465	93.596	1.00 8.06
ATOM	2153	C	TRP	540	56.504	32.189	93.417	1.00 6.24
ATOM	2154	O	TRP	540	56.774	33.366	93.668	1.00 7.32
ATOM	2155	N	GLU	541	55.698	31.467	94.186	1.00 8.81
ATOM	2156	CA	GLU	541	55.187	31.999	95.452	1.00 10.45
ATOM	2157	CB	GLU	541	53.768	32.565	95.270	1.00 11.89
ATOM	2158	CG	GLU	541	53.592	33.523	94.070	1.00 14.89
ATOM	2159	CD	GLU	541	52.202	34.134	93.991	1.00 16.24
ATOM	2160	DE1	GLU	541	52.094	35.229	93.415	1.00 17.33
ATOM	2161	DE2	GLU	541	51.219	33.550	94.516	1.00 16.64
ATOM	2162	C	GLU	541	55.148	30.925	96.507	1.00 10.03
ATOM	2163	O	GLU	541	54.744	29.811	96.232	1.00 10.32
ATOM	2164	N	GLU	542	55.552	31.242	97.724	1.00 10.91
ATOM	2165	CA	GLU	542	55.521	30.222	98.766	1.00 10.78
ATOM	2166	CB	GLU	542	56.871	29.482	98.833	1.00 10.24
ATOM	2167	CG	GLU	542	58.122	30.359	98.738	1.00 14.40
ATOM	2168	CD	GLU	542	59.403	29.571	99.006	1.00 15.97
ATOM	2169	DE1	GLU	542	59.711	29.256	100.188	1.00 17.03
ATOM	2170	DE2	GLU	542	60.095	29.263	98.026	1.00 17.30
ATOM	2171	C	GLU	542	55.083	30.763	100.128	1.00 9.66
ATOM	2172	O	GLU	542	54.741	31.947	100.248	1.00 9.88
ATOM	2173	N	ALA	543	55.051	29.889	101.135	1.00 8.31
ATOM	2174	CA	ALA	543	54.652	30.258	102.493	1.00 7.10
ATOM	2175	CB	ALA	543	54.466	29.038	103.325	1.00 4.26
ATOM	2176	C	ALA	543	55.716	31.141	103.108	1.00 8.66



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ATOM	2177	O	ALA	543	56.911	30.849	102.998	1.00	10.83
ATOM	2178	N	ALA	544	55.286	32.253	103.695	1.00	9.48
ATOM	2179	CA	ALA	544	56.199	33.185	104.325	1.00	10.43
ATOM	2180	CB	ALA	544	55.425	34.374	104.890	1.00	11.53
ATOM	2181	C	ALA	544	56.867	32.397	105.438	1.00	11.84
ATOM	2182	O	ALA	544	56.169	31.744	106.216	1.00	13.61
ATOM	2183	N	SER	545	58.204	32.393	105.456	1.00	12.17
ATOM	2184	CA	SER	545	58.993	31.669	106.453	1.00	13.08
ATOM	2185	CB	SER	545	59.335	30.251	105.980	1.00	12.99
ATOM	2186	OG	SER	545	60.291	29.628	106.827	1.00	14.06
ATOM	2187	C	SER	545	60.245	32.440	106.891	1.00	14.68
ATOM	2188	C	SER	545	60.865	32.184	106.117	1.00	15.67
ATOM	2189	N	ALA	546	60.557	32.271	108.174	1.00	17.50
ATOM	2190	CA	ALA	546	61.639	32.942	108.882	1.00	17.93
ATOM	2191	CB	ALA	546	61.927	32.215	110.200	1.00	17.78
ATOM	2192	C	ALA	546	62.928	33.213	108.143	1.00	18.94
ATOM	2193	O	ALA	546	63.651	32.297	107.751	1.00	19.69
ATOM	2194	N	GLY	547	63.212	34.495	107.965	1.00	19.34
ATOM	2195	CA	GLY	547	64.438	34.889	107.300	1.00	20.46
ATOM	2196	C	GLY	547	64.841	34.140	106.032	1.00	20.86
ATOM	2197	O	GLY	547	66.045	34.046	105.739	1.00	23.71
ATOM	2198	N	VAL	548	63.867	33.560	105.322	1.00	18.62
ATOM	2199	CA	VAL	548	64.111	32.882	104.048	1.00	14.08
ATOM	2200	CB	VAL	548	63.115	31.749	103.826	1.00	12.71
ATOM	2201	CG1	VAL	548	63.134	31.309	102.363	1.00	13.62
ATOM	2202	CG2	VAL	548	63.450	20.579	104.756	1.00	11.28
ATOM	2203	C	VAL	548	63.874	33.971	102.995	1.00	15.33
ATOM	2204	O	VAL	548	62.721	34.309	102.714	1.00	16.13
ATOM	2205	N	GLY	549	64.954	34.612	102.541	1.00	15.42
ATOM	2206	CA	GLY	549	64.852	35.667	101.551	1.00	12.34
ATOM	2207	C	GLY	549	65.473	35.180	100.263	1.00	12.73
ATOM	2208	O	GLY	549	65.765	33.991	100.117	1.00	11.82
ATOM	2209	N	PRO	550	65.666	36.066	99.283	1.00	12.01
ATOM	2210	CD	PRO	550	65.213	37.459	99.186	1.00	12.99
ATOM	2211	CA	PRO	550	66.271	35.639	98.017	1.00	13.59
ATOM	2212	CB	PRO	550	66.333	36.943	97.199	1.00	9.83
ATOM	2213	CG	PRO	550	66.201	38.019	98.199	1.00	10.09
ATOM	2214	C	PRO	550	67.647	34.964	98.157	1.00	13.34
ATOM	2215	O	PRO	550	67.991	34.066	97.377	1.00	14.83
ATOM	2216	N	GLY	551	68.384	35.340	99.204	1.00	13.58
ATOM	2217	CA	GLY	551	69.714	34.797	99.443	1.00	11.00
ATOM	2218	C	GLY	551	69.776	33.300	99.601	1.00	9.01
ATOM	2219	O	GLY	551	70.854	32.736	99.588	1.00	11.57
ATOM	2220	N	ASN	552	68.625	32.655	99.726	1.00	6.84
ATOM	2221	CA	ASN	552	68.573	31.215	99.888	1.00	6.10
ATOM	2222	CB	ASN	552	67.510	30.851	100.904	1.00	4.68
ATOM	2223	CG	ASN	552	67.797	31.449	102.226	1.00	6.53
ATOM	2224	OD1	ASN	552	68.789	31.112	102.850	1.00	7.24
ATOM	2225	ND2	ASN	552	66.991	32.411	102.631	1.00	8.39
ATOM	2226	C	ASN	552	68.287	30.504	98.590	1.00	7.54
ATOM	2227	C	ASN	552	68.176	29.265	98.580	1.00	7.91
ATOM	2228	N	TYR	553	68.157	31.278	97.506	1.00	5.28
ATOM	2229	CA	TYR	553	67.867	30.739	96.186	1.00	4.43
ATOM	2230	CB	TYR	553	66.432	31.088	95.779	1.00	4.87
ATOM	2231	CG	TYR	553	65.367	30.341	95.520	1.00	4.46
ATOM	2232	CD1	TYR	553	64.491	31.001	97.373	1.00	3.71
ATOM	2233	CE1	TYR	553	63.574	30.290	99.117	1.00	3.40
ATOM	2234	CD2	TYR	553	65.280	28.953	95.423	1.00	3.40
ATOM	2235	CE2	TYR	553	64.355	28.243	97.167	1.00	3.44
ATOM	2236	CZ	TYR	553	63.516	28.914	99.012	1.00	2.00
ATOM	2237	OH	TYR	553	62.650	28.189	98.778	1.00	3.67
ATOM	2238	C	TYR	553	68.791	31.287	95.114	1.00	5.08
ATOM	2239	O	TYR	553	69.432	32.306	95.298	1.00	4.35
ATOM	2240	N	SER	554	68.845	30.612	93.980	1.00	5.81
ATOM	2241	CA	SER	554	59.622	31.109	92.865	1.00	6.70
ATOM	2242	CB	SER	554	70.999	30.456	92.932	1.00	8.42
ATOM	2243	OG	SER	554	70.954	29.192	92.214	1.00	11.53
ATOM	2244	C	SER	554	68.800	30.783	91.621	1.00	6.93
ATOM	2245	O	SER	554	68.289	29.584	91.502	1.00	7.53
ATOM	2246	N	PHE	555	68.574	31.733	90.773	1.00	6.48
ATOM	2247	CA	PHE	555	67.811	31.640	89.536	1.00	5.32
ATOM	2248	CB	PHE	555	66.734	32.730	89.484	1.00	5.75
ATOM	2249	CG	PHE	555	65.780	32.591	89.325	1.00	5.98
ATOM	2250	CD1	PHE	555	64.423	32.509	89.567	1.00	3.96
ATOM	2251	CD2	PHE	555	66.242	32.554	87.319	1.00	4.43
ATOM	2252	CE1	PHE	555	63.541	32.382	87.507	1.00	6.29
ATOM	2253	CE2	PHE	555	65.379	32.427	85.963	1.00	3.92
ATOM	2254	CZ	PHE	555	64.030	32.339	85.156	1.00	5.62

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ATOM	2255	C	PHE	555	68.779	31.759	68.337	1.00	6.86	4	
ATOM	2256	O	PHE	555	69.184	32.858	67.945	1.00	8.43	5	
ATOM	2257	N	SER	556	69.095	30.616	67.740	1.00	7.22	7	
ATOM	2258	CA	SER	556	70.019	30.503	66.619	1.00	6.83	4	
ATOM	2259	CB	SER	556	70.969	29.315	66.879	1.00	4.30	5	
ATOM	2260	OG	SER	556	71.923	29.587	67.891	1.00	8.78	5	
ATOM	2261	C	SER	556	69.336	30.298	65.257	1.00	5.62	5	
ATOM	2262	O	SER	556	68.535	29.389	65.117	1.00	8.35	5	
ATOM	2263	N	TYR	557	69.682	31.102	64.255	1.00	3.08	7	
ATOM	2264	CA	TYR	557	69.123	30.943	62.924	1.00	3.30	4	
ATOM	2265	CB	TYR	557	68.198	32.089	62.569	1.00	2.00	5	
ATOM	2266	CG	TYR	557	68.832	33.434	62.422	1.00	2.00	5	
ATOM	2267	CD1	TYR	557	69.405	33.825	61.218	1.00	2.00	6	
ATOM	2268	CE1	TYR	557	69.851	35.126	61.023	1.00	2.56	4	
ATOM	2269	CD2	TYR	557	68.737	34.368	63.434	1.00	2.00	6	
ATOM	2270	CE2	TYR	557	69.184	35.667	63.260	1.00	2.00	6	
ATOM	2271	CZ	TYR	557	69.734	36.047	62.051	1.00	3.10	6	
ATOM	2272	OH	TYR	557	70.124	37.356	61.865	1.00	3.23	5	
ATOM	2273	C	TYR	557	70.191	30.834	61.870	1.00	3.33	4	
ATOM	2274	O	TYR	557	71.316	31.196	62.090	1.00	4.25	5	
ATOM	2275	N	GLN	558	69.839	30.360	60.695	1.00	3.52	7	
ATOM	2276	CA	GLN	558	70.831	30.227	59.648	1.00	3.20	4	
ATOM	2277	CB	GLN	558	71.603	28.925	59.828	1.00	3.66	4	
ATOM	2278	CG	GLN	558	72.506	28.598	58.648	1.00	6.55	4	
ATOM	2279	CD	GLN	558	73.171	27.282	58.788	1.00	5.14	4	
ATOM	2280	OE1	GLN	558	72.552	26.320	59.163	1.00	6.68	5	
ATOM	2281	NE2	GLN	558	74.447	27.229	58.477	1.00	7.23	7	
ATOM	2282	C	GLN	558	70.204	30.208	58.279	1.00	3.24	4	
ATOM	2283	O	GLN	558	69.420	29.309	57.977	1.00	2.96	5	
ATOM	2284	N	LEU	559	70.518	31.189	57.445	1.00	2.00	7	
ATOM	2285	CA	LEU	559	69.945	31.139	56.120	1.00	2.89	5	
ATOM	2286	CB	LEU	559	70.036	32.487	55.399	1.00	2.00	4	
ATOM	2287	CG	LEU	559	68.975	33.527	55.792	1.00	2.00	6	
ATOM	2288	CD1	LEU	559	69.103	34.810	55.005	1.00	2.00	6	
ATOM	2289	CD2	LEU	559	67.612	32.955	55.564	1.00	2.00	6	
ATOM	2290	C	LEU	559	70.764	30.060	55.447	1.00	5.30	6	
ATOM	2291	O	LEU	559	71.951	29.947	55.728	1.00	4.67	5	
ATOM	2292	N	GLU	560	70.091	29.169	54.718	1.00	6.97	7	
ATOM	2293	CA	GLU	560	70.737	28.064	53.997	1.00	11.03	6	
ATOM	2294	CB	GLU	560	69.787	27.517	52.938	1.00	14.40	4	
ATOM	2295	CG	GLU	560	70.290	26.305	52.163	1.00	19.08	5	
ATOM	2296	CD	GLU	560	69.701	26.207	50.738	1.00	20.20	4	
ATOM	2297	OE1	GLU	560	69.790	27.202	49.983	1.00	25.39	5	
ATOM	2298	OE2	GLU	560	69.200	25.130	50.346	1.00	21.83	5	
ATOM	2299	C	GLU	560	71.995	28.572	53.310	1.00	11.71	4	
ATOM	2300	O	GLU	560	71.919	29.491	52.505	1.00	10.88	5	
ATOM	2301	N	ASP	561	73.140	27.970	53.648	1.00	12.36	7	
ATOM	2302	CA	ASP	561	74.460	28.346	53.118	1.00	13.20	4	
ATOM	2303	CB	ASP	561	74.478	28.398	51.589	1.00	11.29	4	
ATOM	2304	CG	ASP	561	74.440	27.038	50.968	1.00	13.29	4	
ATOM	2305	OD1	ASP	561	74.530	26.039	51.725	1.00	14.53	5	
ATOM	2306	OD2	ASP	561	74.296	26.963	49.729	1.00	11.84	5	
ATOM	2307	C	ASP	561	74.995	29.667	53.661	1.00	17.27	4	
ATOM	2308	O	ASP	561	75.663	30.426	52.931	1.00	21.27	5	
ATOM	2309	N	GLU	562	74.714	29.972	54.926	1.00	17.40	7	
ATOM	2310	CA	GLU	562	75.220	31.218	55.504	1.00	16.45	4	
ATOM	2311	CB	GLU	562	74.093	32.235	55.652	1.00	20.22	4	
ATOM	2312	CG	GLU	562	73.224	32.450	54.408	1.00	23.17	5	
ATOM	2313	CD	GLU	562	73.909	33.234	53.289	1.00	23.82	4	
ATOM	2314	OE1	GLU	562	74.330	34.407	53.511	1.00	22.18	5	
ATOM	2315	OE2	GLU	562	73.981	32.670	52.169	1.00	27.47	5	
ATOM	2316	C	GLU	562	75.764	30.847	55.871	1.00	14.28	5	
ATOM	2317	O	GLU	562	75.431	29.759	55.373	1.00	15.04	5	
ATOM	2318	N	PRO	563	76.662	31.681	55.465	1.00	11.29	7	
ATOM	2319	CD	PRO	563	77.200	32.000	55.084	1.00	8.24	7	
ATOM	2320	CA	PRO	563	77.156	31.287	53.794	1.00	11.69	5	
ATOM	2321	CB	PRO	563	78.186	32.376	53.111	1.00	7.10	5	
ATOM	2322	CG	PRO	563	77.655	33.548	54.404	1.00	6.79	5	
ATOM	2323	C	PRO	563	75.965	31.277	53.788	1.00	10.73	5	
ATOM	2324	O	PRO	563	74.981	32.001	53.558	1.00	11.06	5	
ATOM	2325	N	TRP	564	75.995	30.362	60.772	1.00	8.20	7	
ATOM	2326	CA	TRP	564	74.945	30.255	61.806	1.00	5.30	4	
ATOM	2327	CB	TRP	564	75.304	29.199	62.845	1.00	2.55	5	
ATOM	2328	CG	TRP	564	74.650	27.886	62.700	1.00	5.08	5	
ATOM	2329	CD2	TRP	564	73.276	27.585	62.941	1.00	6.62	5	
ATOM	2330	CE2	TRP	564	73.116	26.182	62.761	1.00	6.36	5	
ATOM	2331	CE1	TRP	564	72.158	28.357	63.296	1.00	8.59	5	
ATOM	2332	CD1	TRP	564	75.250	26.700	62.387	1.00	6.26	5	

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ATOM	2333	NE1	TRP	564	74.332	25.675	82.422	1.00	5.56	7
ATOM	2334	CZ2	TRP	564	71.880	25.346	82.929	1.00	6.49	7
ATOM	2335	CZ3	TRP	564	70.928	27.723	83.461	1.00	6.79	7
ATOM	2336	CH2	TRP	564	70.801	26.328	83.279	1.00	8.18	7
ATOM	2337	C	TRP	564	74.880	31.597	82.525	1.00	5.66	7
ATOM	2338	C	TRP	564	75.908	32.259	82.740	1.00	9.32	7
ATOM	2339	N	LYS	565	73.690	31.997	82.927	1.00	3.69	7
ATOM	2340	CA	LYS	565	73.542	33.256	83.612	1.00	2.30	7
ATOM	2341	CB	LYS	565	73.099	34.332	82.625	1.00	2.00	7
ATOM	2342	CG	LYS	565	74.242	34.886	81.791	1.00	2.00	7
ATOM	2343	CD	LYS	565	73.827	35.197	80.371	1.00	3.81	7
ATOM	2344	CE	LYS	565	74.814	36.116	79.711	1.00	3.15	7
ATOM	2345	NZ	LYS	565	74.856	37.374	80.497	1.00	6.31	7
ATOM	2346	C	LYS	565	72.669	33.171	84.878	1.00	3.24	7
ATOM	2347	O	LYS	565	71.856	32.270	85.043	1.00	2.93	7
ATOM	2348	N	LEU	566	72.863	34.113	85.783	1.00	3.46	7
ATOM	2349	CA	LEU	566	72.160	34.100	87.042	1.00	6.16	7
ATOM	2350	CB	LEU	566	73.187	33.857	88.143	1.00	7.13	7
ATOM	2351	CG	LEU	566	72.902	33.890	89.641	1.00	11.04	7
ATOM	2352	CD1	LEU	566	74.121	33.292	90.343	1.00	13.73	7
ATOM	2353	CD2	LEU	566	72.660	35.299	90.155	1.00	11.29	7
ATOM	2354	C	LEU	566	71.305	35.418	87.265	1.00	6.69	7
ATOM	2355	C	LEU	566	72.175	36.430	87.315	1.00	6.50	7
ATOM	2356	N	CYS	567	70.199	35.446	87.406	1.00	7.27	7
ATOM	2357	CA	CYS	567	69.636	36.738	87.658	1.00	10.38	7
ATOM	2358	C	CYS	567	69.245	37.013	89.124	1.00	13.50	7
ATOM	2359	O	CYS	567	69.271	36.113	89.983	1.00	13.64	7
ATOM	2360	CB	CYS	567	68.506	37.017	86.707	1.00	12.07	7
ATOM	2361	SG	CYS	567	67.190	35.797	86.808	1.00	17.22	7
ATOM	2362	N	ARG	568	69.009	38.293	89.405	1.00	15.13	7
ATOM	2363	CA	ARG	568	68.626	38.777	90.727	1.00	14.78	7
ATOM	2364	CB	ARG	568	68.781	40.310	90.798	1.00	17.37	7
ATOM	2365	CG	ARG	568	70.037	40.829	91.510	1.00	20.45	7
ATOM	2366	CD	ARG	568	71.329	40.711	90.681	1.00	20.67	7
ATOM	2367	NE	ARG	568	72.045	41.996	90.624	1.00	22.26	7
ATOM	2368	CZ	ARG	568	72.587	42.642	91.671	1.00	22.85	7
ATOM	2369	NH1	ARG	568	72.531	42.151	92.918	1.00	20.25	7
ATOM	2370	NH2	ARG	568	73.191	43.816	91.465	1.00	24.23	7
ATOM	2371	C	ARG	568	67.185	38.399	91.086	1.00	14.39	7
ATOM	2372	O	ARG	568	66.247	38.690	90.329	1.00	15.75	7
ATOM	2373	N	LEU	569	67.046	37.752	92.248	1.00	11.39	7
ATOM	2374	CA	LEU	569	65.782	37.304	92.807	1.00	6.92	7
ATOM	2375	CB	LEU	569	66.005	36.101	93.715	1.00	2.00	7
ATOM	2376	CG	LEU	569	65.069	34.917	93.607	1.00	3.41	7
ATOM	2377	CD1	LEU	569	64.374	34.905	92.287	1.00	3.80	7
ATOM	2378	CD2	LEU	569	65.852	33.675	93.759	1.00	2.00	7
ATOM	2379	C	LEU	569	65.318	36.461	93.637	1.00	7.64	7
ATOM	2380	O	LEU	569	66.121	39.228	94.131	1.00	6.24	7
ATOM	2381	N	HIS	570	64.015	38.644	93.719	1.00	9.65	7
ATOM	2382	CA	HIS	570	63.454	39.712	94.531	1.00	10.84	7
ATOM	2383	CB	HIS	570	62.841	40.811	93.655	1.00	11.04	7
ATOM	2384	CG	HIS	570	63.820	41.547	92.802	1.00	10.31	7
ATOM	2385	CD2	HIS	570	64.739	42.492	93.109	1.00	12.10	7
ATOM	2386	ND1	HIS	570	63.845	41.421	91.431	1.00	14.00	7
ATOM	2387	CE1	HIS	570	64.728	42.263	90.925	1.00	14.17	7
ATOM	2388	NE2	HIS	570	65.285	42.925	91.924	1.00	12.65	7
ATOM	2389	C	HIS	570	62.359	39.076	95.393	1.00	9.92	7
ATOM	2390	O	HIS	570	62.098	37.884	95.284	1.00	14.44	7
ATOM	2391	N	GLN	571	61.725	39.869	96.246	1.00	9.24	7
ATOM	2392	CA	GLN	571	60.655	39.369	97.063	1.00	6.37	7
ATOM	2393	CB	GLN	571	61.187	38.806	98.371	1.00	11.43	7
ATOM	2394	CG	GLN	571	60.150	38.017	99.168	1.00	19.07	7
ATOM	2395	CD	GLN	571	60.187	38.342	100.666	1.00	21.53	7
ATOM	2396	OE1	GLN	571	61.169	38.037	101.358	1.00	22.69	7
ATOM	2397	NE2	GLN	571	59.116	38.962	101.170	1.00	22.76	7
ATOM	2398	C	GLN	571	59.712	40.504	97.308	1.00	1.52	7
ATOM	2399	O	GLN	571	60.098	41.656	97.285	1.00	2.00	7
ATOM	2400	N	ALA	572	58.445	40.152	97.419	1.00	4.26	7
ATOM	2401	CA	ALA	572	57.348	41.081	97.656	1.00	5.12	7
ATOM	2402	CB	ALA	572	56.920	41.774	96.356	1.00	2.27	7
ATOM	2403	C	ALA	572	56.217	40.214	98.195	1.00	4.95	7
ATOM	2404	O	ALA	572	56.260	38.974	98.057	1.00	6.25	7
ATOM	2405	N	PRO	573	55.213	40.327	98.864	1.00	9.54	7
ATOM	2406	CD	PRO	573	55.084	42.102	99.602	1.00	6.45	7
ATOM	2407	CA	PRO	573	54.205	39.868	99.323	1.00	8.15	7
ATOM	2408	CB	PRO	573	53.769	40.437	100.696	1.00	9.62	7
ATOM	2409	CG	PRO	573	54.785	41.599	100.984	1.00	7.39	7
ATOM	2410	C	PRO	573	53.044	39.724	99.377	1.00	7.53	7

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ATOM	2411	O	PRO	573	52.768	40.608	97.552	1.00	7.72	3
ATOM	2412	N	THR	574	52.428	38.574	98.476	1.00	8.95	7
ATOM	2413	CA	THR	574	51.255	38.232	97.727	1.00	10.96	6
ATOM	2414	CB	THR	574	51.075	36.738	97.733	1.00	10.37	6
ATOM	2415	OG1	THR	574	52.135	36.153	96.980	1.00	14.24	3
ATOM	2416	CG2	THR	574	49.712	36.324	97.155	1.00	13.72	6
ATOM	2417	C	THR	574	50.119	38.852	98.515	1.00	12.85	6
ATOM	2418	O	THR	574	50.163	38.874	99.753	1.00	14.59	3
ATOM	2419	N	ALA	575	49.087	39.324	97.812	1.00	14.88	7
ATOM	2420	CA	ALA	575	47.934	39.946	98.467	1.00	14.50	6
ATOM	2421	CB	ALA	575	46.932	40.433	97.439	1.00	14.72	5
ATOM	2422	C	ALA	575	47.282	38.960	99.443	1.00	14.38	5
ATOM	2423	O	ALA	575	46.480	39.355	100.286	1.00	15.91	3
ATOM	2424	N	ARG	576	47.663	37.695	99.344	1.00	12.79	7
ATOM	2425	CA	ARG	576	47.176	36.637	100.189	1.00	11.82	6
ATOM	2426	CB	ARG	576	46.877	35.414	99.328	1.00	15.95	6
ATOM	2427	CG	ARG	576	45.534	35.451	98.604	1.00	20.92	6
ATOM	2428	CD	ARG	576	45.633	34.631	97.302	1.00	24.61	6
ATOM	2429	NE	ARG	576	44.350	34.081	96.848	1.00	27.37	7
ATOM	2430	CZ	ARG	576	44.171	33.438	95.687	1.00	28.99	6
ATOM	2431	NH1	ARG	576	45.188	33.261	94.833	1.00	29.46	7
ATOM	2432	NH2	ARG	576	42.979	32.928	95.391	1.00	27.90	7
ATOM	2433	C	ARG	576	48.090	36.216	101.351	1.00	9.90	5
ATOM	2434	O	ARG	576	47.843	35.177	101.972	1.00	8.14	5
ATOM	2435	N	GLY	577	49.167	36.963	101.606	1.00	10.36	7
ATOM	2436	CA	GLY	577	50.066	36.615	102.705	1.00	9.58	6
ATOM	2437	C	GLY	577	51.201	35.638	102.435	1.00	11.02	6
ATOM	2438	O	GLY	577	51.959	35.280	103.356	1.00	10.42	5
ATOM	2439	N	ALA	578	51.263	35.140	101.193	1.00	11.51	7
ATOM	2440	CA	ALA	578	52.332	34.245	100.730	1.00	10.32	6
ATOM	2441	CB	ALA	578	51.842	33.360	99.617	1.00	6.95	5
ATOM	2442	C	ALA	578	53.443	35.158	100.212	1.00	10.21	6
ATOM	2443	O	ALA	578	53.278	36.384	100.138	1.00	9.88	8
ATOM	2444	N	VAL	579	54.597	34.593	99.905	1.00	9.95	7
ATOM	2445	CA	VAL	579	55.673	35.431	99.406	1.00	10.55	6
ATOM	2446	CB	VAL	579	56.957	35.294	100.247	1.00	9.32	6
ATOM	2447	CG1	VAL	579	56.734	35.863	101.618	1.00	8.45	6
ATOM	2448	CG2	VAL	579	57.363	33.860	100.350	1.00	11.44	6
ATOM	2449	C	VAL	579	55.922	35.128	97.939	1.00	9.09	5
ATOM	2450	O	VAL	579	55.599	34.044	97.452	1.00	8.40	5
ATOM	2451	N	ARG	580	56.460	36.104	97.229	1.00	7.06	7
ATOM	2452	CA	ARG	580	56.721	35.917	95.816	1.00	7.86	6
ATOM	2453	CB	ARG	580	55.769	36.792	94.991	1.00	8.84	6
ATOM	2454	CG	ARG	580	55.926	36.721	93.503	1.00	7.88	6
ATOM	2455	CD	ARG	580	55.080	37.813	92.844	1.00	8.78	5
ATOM	2456	NE	ARG	580	53.652	37.517	92.913	1.00	6.85	7
ATOM	2457	CZ	ARG	580	52.719	36.362	93.341	1.00	5.69	5
ATOM	2458	NH1	ARG	580	53.050	39.581	93.731	1.00	5.12	7
ATOM	2459	NH2	ARG	580	51.470	37.952	93.466	1.00	2.00	7
ATOM	2460	C	ARG	580	58.159	36.282	95.523	1.00	7.72	5
ATOM	2461	O	ARG	580	58.664	37.321	95.954	1.00	7.66	5
ATOM	2462	N	PHE	581	58.827	35.387	94.827	1.00	6.07	7
ATOM	2463	CA	PHE	581	60.200	35.596	94.458	1.00	5.52	5
ATOM	2464	CB	PHE	581	60.982	34.355	94.803	1.00	4.84	5
ATOM	2465	CG	PHE	581	61.274	34.214	96.250	1.00	4.90	5
ATOM	2466	CD1	PHE	581	60.510	22.372	97.045	1.00	3.60	5
ATOM	2467	CD2	PHE	581	62.371	34.883	96.822	1.00	5.69	5
ATOM	2468	CE1	PHE	581	60.835	33.191	98.390	1.00	4.44	5
ATOM	2469	CE2	PHE	581	62.694	34.700	98.165	1.00	5.88	5
ATOM	2470	CZ	PHE	581	61.926	33.854	98.944	1.00	3.43	5
ATOM	2471	C	PHE	581	60.287	35.839	92.961	1.00	5.46	5
ATOM	2472	O	PHE	581	59.686	35.101	92.194	1.00	6.33	5
ATOM	2473	N	TRP	582	61.037	36.844	92.525	1.00	6.16	7
ATOM	2474	CA	TRP	582	61.129	37.054	91.090	1.00	7.26	5
ATOM	2475	CB	TRP	582	59.861	37.778	90.589	1.00	9.34	5
ATOM	2476	CG	TRP	582	59.462	38.933	91.423	1.00	10.74	5
ATOM	2477	CD2	TRP	582	59.916	40.268	91.280	1.00	11.49	5
ATOM	2478	CE2	TRP	582	59.366	41.017	92.359	1.00	11.22	5
ATOM	2479	CE3	TRP	582	60.744	40.906	90.356	1.00	11.65	5
ATOM	2480	CD1	TRP	582	58.665	38.915	92.530	1.00	14.19	5
ATOM	2481	NE1	TRP	582	58.604	40.165	93.105	1.00	12.18	7
ATOM	2482	CZ2	TRP	582	59.616	42.365	92.538	1.00	12.31	5
ATOM	2483	CZ3	TRP	582	61.001	42.247	90.524	1.00	15.91	5
ATOM	2484	CH2	TRP	582	60.436	42.973	91.657	1.00	16.33	5
ATOM	2485	C	TRP	582	62.409	37.522	90.429	1.00	7.94	5
ATOM	2486	O	TRP	582	63.219	38.299	91.041	1.00	6.37	5
ATOM	2487	N	CYS	583	62.556	37.312	89.150	1.00	7.90	7
ATOM	2488	CA	CYS	583	63.658	37.766	89.334	1.00	9.15	5

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ATOM	2489	C	CYS	583	63.154	38.449	87.073	1.00	8.52	5
ATOM	2490	O	CYS	583	62.143	38.055	86.520	1.00	8.13	3
ATOM	2491	CB	CYS	583	64.507	36.591	87.876	1.00	11.02	5
ATOM	2492	SG	CYS	583	65.603	36.996	85.470	1.00	12.88	15
ATOM	2493	N	SER	584	63.895	39.453	86.606	1.00	11.08	7
ATOM	2494	CA	SER	584	63.556	40.150	85.375	1.00	11.13	5
ATOM	2495	CB	SER	584	63.210	41.612	85.649	1.00	14.00	5
ATOM	2496	OG	SER	584	62.296	42.141	84.680	1.00	22.72	5
ATOM	2497	C	SER	584	64.819	40.052	84.531	1.00	11.03	5
ATOM	2498	O	SER	584	65.874	40.485	84.990	1.00	14.12	5
ATOM	2499	N	LEU	585	64.743	39.357	83.390	1.00	8.82	7
ATOM	2500	CA	LEU	585	65.889	39.214	82.500	1.00	7.31	5
ATOM	2501	CB	LEU	585	65.638	38.192	81.374	1.00	5.24	5
ATOM	2502	CG	LEU	585	65.265	36.731	81.541	1.00	2.00	5
ATOM	2503	CD1	LEU	585	65.929	35.888	80.486	1.00	2.00	5
ATOM	2504	CD2	LEU	585	65.633	36.271	82.912	1.00	5.67	5
ATOM	2505	C	LEU	585	66.134	40.562	81.832	1.00	8.79	5
ATOM	2506	O	LEU	585	65.188	41.282	81.508	1.00	7.56	3
ATOM	2507	N	PRO	586	67.410	40.929	81.637	1.00	10.50	7
ATOM	2508	CD	PRO	586	68.622	40.279	82.160	1.00	12.29	6
ATOM	2509	CA	PRO	586	67.746	42.202	80.993	1.00	11.85	5
ATOM	2510	CB	PRO	586	69.257	42.304	81.191	1.00	11.45	5
ATOM	2511	CG	PRO	586	69.505	41.470	82.416	1.00	13.83	5
ATOM	2512	C	PRO	586	67.416	42.019	79.520	1.00	14.14	6
ATOM	2513	O	PRO	586	67.834	41.019	78.912	1.00	14.17	8
ATOM	2514	N	THR	587	66.691	42.985	78.957	1.00	13.17	7
ATOM	2515	CA	THR	587	66.261	42.949	77.569	1.00	12.49	5
ATOM	2516	CB	THR	587	66.168	44.355	76.969	1.00	15.17	5
ATOM	2517	OG1	THR	587	65.927	45.330	78.002	1.00	18.67	5
ATOM	2518	CG2	THR	587	65.049	44.408	75.929	1.00	17.05	6
ATOM	2519	C	THR	587	67.182	42.186	76.657	1.00	12.00	6
ATOM	2520	O	THR	587	66.739	41.308	75.948	1.00	11.83	8
ATOM	2521	N	ALA	588	68.472	42.530	76.700	1.00	11.51	7
ATOM	2522	CA	ALA	588	69.512	41.927	75.849	1.00	7.86	6
ATOM	2523	CB	ALA	588	70.896	42.342	76.320	1.00	8.95	6
ATOM	2524	C	ALA	588	69.435	40.425	75.700	1.00	7.36	5
ATOM	2525	O	ALA	588	69.825	39.894	74.681	1.00	8.37	3
ATOM	2526	N	ASP	589	68.877	39.747	76.693	1.00	7.82	7
ATOM	2527	CA	ASP	589	68.745	38.300	76.651	1.00	7.85	5
ATOM	2528	CB	ASP	589	69.173	37.684	77.976	1.00	5.24	5
ATOM	2529	CG	ASP	589	70.673	37.683	78.168	1.00	5.26	5
ATOM	2530	OD1	ASP	589	71.088	38.045	79.298	1.00	6.38	5
ATOM	2531	OD2	ASF	589	71.422	37.299	77.230	1.00	2.00	5
ATOM	2532	C	ASF	589	67.341	37.845	76.376	1.00	7.96	5
ATOM	2533	O	ASP	589	67.080	36.659	76.383	1.00	7.86	5
ATOM	2534	N	THR	590	66.435	38.780	76.133	1.00	8.88	7
ATOM	2535	CA	THR	590	65.040	38.451	75.899	1.00	10.02	5
ATOM	2536	CS	THR	590	64.118	39.571	76.426	1.00	8.46	5
ATOM	2537	OG1	THR	590	64.496	40.806	75.845	1.00	7.66	3
ATOM	2538	CG2	THR	590	64.269	39.728	77.928	1.00	10.59	5
ATOM	2539	C	THR	590	64.696	38.106	74.465	1.00	10.88	5
ATOM	2540	O	THR	590	63.610	38.414	74.007	1.00	15.28	5
ATOM	2541	N	SER	591	65.592	37.405	73.783	1.00	11.68	7
ATOM	2542	CA	SER	591	65.372	37.022	72.391	1.00	11.91	5
ATOM	2543	CB	SER	591	66.692	36.681	71.696	1.00	13.98	5
ATOM	2544	OG	SER	591	67.046	37.715	70.790	1.00	16.79	5
ATOM	2545	C	SER	591	64.405	35.867	72.177	1.00	11.64	5
ATOM	2546	O	SER	591	64.456	34.847	72.882	1.00	12.56	5
ATOM	2547	N	SER	592	63.585	35.999	71.135	1.00	9.34	5
ATOM	2548	CA	SER	592	62.607	34.988	70.803	1.00	5.84	5
ATOM	2549	CB	SER	592	61.395	35.633	70.119	1.00	6.26	5
ATOM	2550	OG	SER	592	60.795	36.638	70.916	1.00	5.45	5
ATOM	2551	C	SER	592	63.216	33.945	69.669	1.00	5.35	5
ATOM	2552	C	SER	592	64.386	32.974	69.563	1.00	4.72	5
ATOM	2553	N	PHE	593	62.388	32.980	69.527	1.00	5.79	7
ATOM	2554	CA	PHE	593	62.715	31.900	68.620	1.00	8.33	5
ATOM	2555	CB	PHE	593	62.866	32.474	67.189	1.00	7.57	5
ATOM	2556	CG	PHE	593	61.744	33.458	66.791	1.00	6.76	5
ATOM	2557	CD1	PHE	593	62.041	34.679	66.167	1.00	9.27	5
ATOM	2558	CD2	PHE	593	60.399	33.162	67.043	1.00	5.21	5
ATOM	2559	CE1	PHE	593	61.020	35.584	65.866	1.00	9.60	5
ATOM	2560	CE2	PHE	593	59.380	34.054	65.719	1.00	5.01	5
ATOM	2561	CD	PHE	593	59.686	35.262	65.121	1.00	7.44	5
ATOM	2562	C	PHE	593	63.848	30.947	69.000	1.00	9.84	5
ATOM	2563	O	PHE	593	64.302	30.177	68.151	1.00	11.09	5
ATOM	2564	N	VAL	594	64.223	30.958	70.291	1.00	9.82	5
ATOM	2565	CA	VAL	594	65.284	30.113	70.891	1.00	8.29	5
ATOM	2566	CB	VAL	594	66.588	30.909	71.155	1.00	9.17	5

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ATOM	2567	CG1 VAL	594	67.086	31.490	69.894	1.00	11.27
ATOM	2568	CG2 VAL	594	66.359	32.005	72.175	1.00	8.98
ATOM	2569	C VAL	594	64.874	29.552	72.261	1.00	6.86
ATOM	2570	O VAL	594	64.201	30.239	73.037	1.00	9.44
ATOM	2571	N PRO	595	65.287	28.308	72.572	1.00	4.06
ATOM	2572	CD PRO	595	65.910	27.414	71.592	1.00	4.50
ATOM	2573	CA PRO	595	65.040	27.558	73.802	1.00	4.33
ATOM	2574	CB PRO	595	65.623	26.185	73.468	1.00	4.07
ATOM	2575	CG PRO	595	65.442	26.084	72.064	1.00	2.00
ATOM	2576	C PRO	595	65.728	26.142	75.048	1.00	3.58
ATOM	2577	O PRO	595	66.955	28.077	75.180	1.00	3.03
ATOM	2578	N LEU	596	64.923	28.692	75.955	1.00	3.21
ATOM	2579	CA LEU	596	65.420	29.282	77.199	1.00	4.16
ATOM	2580	CB LEU	596	64.670	30.596	77.561	1.00	3.29
ATOM	2581	CG LEU	596	65.384	31.870	78.068	1.00	2.00
ATOM	2582	CD1 LEU	596	64.500	32.639	79.002	1.00	3.47
ATOM	2583	CD2 LEU	596	66.646	31.534	78.783	1.00	2.16
ATOM	2584	C LEU	596	65.252	28.293	78.347	1.00	4.67
ATOM	2585	O LEU	596	64.121	27.938	78.721	1.00	2.52
ATOM	2586	N GLU	597	66.384	27.861	78.900	1.00	4.53
ATOM	2587	CA GLU	597	66.406	26.943	80.031	1.00	3.76
ATOM	2588	CB GLU	597	67.566	25.980	79.909	1.00	2.00
ATOM	2589	CG GLU	597	67.699	25.125	81.113	1.00	2.00
ATOM	2590	CD GLU	597	68.548	23.955	80.855	1.00	5.62
ATOM	2591	OE1 GLU	597	69.206	23.971	79.805	1.00	10.01
ATOM	2592	OE2 GLU	597	68.562	22.014	81.675	1.00	6.65
ATOM	2593	C GLU	597	66.483	27.704	81.367	1.00	2.57
ATOM	2594	O GLU	597	67.322	28.596	81.536	1.00	3.19
ATOM	2595	N LEU	598	65.590	27.358	82.296	1.00	3.03
ATOM	2596	CA LEU	598	65.519	28.001	83.600	1.00	2.16
ATOM	2597	CB LEU	598	64.159	28.670	83.777	1.00	2.00
ATOM	2598	CG LEU	598	63.756	29.657	82.681	1.00	2.00
ATOM	2599	CD1 LEU	598	62.279	29.702	82.601	1.00	2.00
ATOM	2600	CD2 LEU	598	64.368	31.027	82.888	1.00	2.00
ATOM	2601	C LEU	598	65.761	26.988	84.700	1.00	2.92
ATOM	2602	O LEU	598	65.337	25.833	84.605	1.00	2.64
ATOM	2603	N ARG	599	66.462	27.428	85.736	1.00	2.34
ATOM	2604	CA ARG	599	66.804	26.580	86.862	1.00	3.62
ATOM	2605	CB ARG	599	68.254	26.115	86.710	1.00	6.78
ATOM	2606	CG ARG	599	68.479	24.611	86.512	1.00	10.90
ATOM	2607	CD ARG	599	69.385	24.359	85.308	1.00	14.84
ATOM	2608	NE ARG	599	69.658	22.945	85.047	1.00	17.19
ATOM	2609	C2 ARG	599	70.176	22.100	85.942	1.00	17.80
ATOM	2610	NH1 ARG	599	70.472	22.515	87.182	1.00	17.23
ATOM	2611	NH2 ARG	599	70.452	20.845	85.580	1.00	15.70
ATOM	2612	C ARG	599	66.717	27.367	88.150	1.00	3.41
ATOM	2613	O ARG	599	67.394	28.364	88.259	1.00	4.23
ATOM	2614	N VAL	600	65.843	26.979	89.081	1.00	2.87
ATOM	2615	CA VAL	600	65.756	27.644	90.387	1.00	2.37
ATOM	2616	CB VAL	600	64.322	28.001	90.825	1.00	2.02
ATOM	2617	CG1 VAL	600	64.336	28.512	92.248	1.00	2.00
ATOM	2618	CG2 VAL	600	63.737	29.035	89.917	1.00	2.00
ATOM	2619	C VAL	600	66.273	26.622	91.371	1.00	3.23
ATOM	2620	O VAL	600	65.744	25.525	91.426	1.00	4.11
ATOM	2621	N THR	601	67.309	26.963	92.124	1.00	5.21
ATOM	2622	CA THR	601	67.881	26.043	93.098	1.00	6.74
ATOM	2623	CB THR	601	69.296	25.601	92.688	1.00	8.50
ATOM	2624	OG1 THR	601	69.228	24.939	91.430	1.00	12.77
ATOM	2625	CG2 THR	601	69.890	24.631	93.684	1.00	8.70
ATOM	2626	C THR	601	67.995	26.634	94.481	1.00	8.74
ATOM	2627	O THR	601	68.267	27.822	94.637	1.00	11.77
ATOM	2628	N ALA	602	67.788	25.792	95.484	1.00	9.57
ATOM	2629	CA ALA	602	67.915	26.196	96.877	1.00	9.62
ATOM	2630	CB ALA	602	67.254	25.191	97.745	1.00	3.55
ATOM	2631	C ALA	602	69.404	26.180	97.153	1.00	10.39
ATOM	2632	O ALA	602	70.107	25.324	96.613	1.00	11.86
ATOM	2633	N ALA	603	69.872	27.069	98.036	1.00	9.75
ATOM	2634	CA ALA	603	71.292	27.162	98.415	1.00	7.23
ATOM	2635	CB ALA	603	71.517	28.370	99.300	1.00	6.77
ATOM	2636	C ALA	603	71.871	25.882	99.070	1.00	5.23
ATOM	2637	O ALA	603	73.066	25.785	99.320	1.00	4.90
ATOM	2638	N SER	604	71.026	24.892	99.324	1.00	5.87
ATOM	2639	CA SER	604	71.497	23.639	99.897	1.00	7.44
ATOM	2640	CB SER	604	70.409	22.980	100.740	1.00	6.37
ATOM	2641	OG SER	604	69.702	22.024	99.997	1.00	5.42
ATOM	2642	C SER	604	71.914	22.689	98.777	1.00	9.15
ATOM	2643	O SER	604	72.462	21.617	99.042	1.00	11.68
ATOM	2644	N GLY	605	71.604	23.070	97.535	1.00	9.29

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ATOM	2645	CA	GLY	605	71.944	22.262	56.378	1.00	8.17
ATOM	2646	C	GLY	605	70.709	21.620	55.785	1.00	7.43
ATOM	2647	O	GLY	605	70.711	21.198	94.631	1.00	8.81
ATOM	2648	N	ALA	606	69.639	21.606	56.572	1.00	7.11
ATOM	2649	CA	ALA	606	68.376	21.001	96.194	1.00	6.20
ATOM	2650	CB	ALA	606	67.492	20.885	97.387	1.00	2.64
ATOM	2651	C	ALA	606	67.665	21.770	95.112	1.00	6.88
ATOM	2652	O	ALA	606	67.450	22.974	95.234	1.00	7.80
ATOM	2653	N	PRO	607	67.222	21.063	94.074	1.00	6.21
ATOM	2654	CD	PRO	607	67.457	19.636	93.821	1.00	6.78
ATOM	2655	CA	PRO	607	66.520	21.660	92.950	1.00	7.75
ATOM	2656	CB	PRO	607	66.656	20.587	91.845	1.00	7.27
ATOM	2657	CG	PRO	607	67.655	19.620	92.355	1.00	5.40
ATOM	2658	C	PRO	607	65.046	21.969	93.220	1.00	6.86
ATOM	2659	O	PRO	607	64.287	21.084	93.599	1.00	6.25
ATOM	2660	N	ARG	608	64.656	23.215	92.953	1.00	6.55
ATOM	2661	CA	ARG	608	63.284	23.658	93.095	1.00	6.82
ATOM	2662	CB	ARG	608	63.198	25.105	93.591	1.00	7.55
ATOM	2663	CG	ARG	608	63.510	25.320	95.066	1.00	11.99
ATOM	2664	CD	ARG	608	62.608	24.474	95.992	1.00	14.22
ATOM	2665	NE	ARG	608	61.169	24.719	95.820	1.00	14.28
ATOM	2666	CZ	ARG	608	60.530	25.828	96.200	1.00	14.39
ATOM	2667	NH1	ARG	608	61.193	26.817	96.773	1.00	15.96
ATOM	2668	NH2	ARG	608	59.216	25.936	96.048	1.00	13.38
ATOM	2669	C	ARG	608	62.586	23.548	91.739	1.00	6.91
ATOM	2670	O	ARG	608	61.613	22.836	91.612	1.00	8.99
ATOM	2671	N	TYR	609	63.095	24.194	90.700	1.00	7.03
ATOM	2672	CA	TYR	609	62.405	24.140	89.406	1.00	7.82
ATOM	2673	CB	TYR	609	61.532	25.394	89.203	1.00	9.92
ATOM	2674	CG	TYR	609	60.543	25.684	90.298	1.00	11.75
ATOM	2675	CD1	TYR	609	60.700	26.798	91.137	1.00	12.36
ATOM	2676	CE1	TYR	609	59.768	27.078	92.156	1.00	13.98
ATOM	2677	CD2	TYR	609	59.434	24.852	90.499	1.00	13.86
ATOM	2678	CE2	TYR	609	58.494	25.120	91.506	1.00	13.63
ATOM	2679	CZ	TYR	609	58.664	26.235	92.326	1.00	15.21
ATOM	2680	OH	TYR	609	57.689	26.529	93.255	1.00	17.36
ATOM	2681	C	TYR	609	63.316	24.032	88.193	1.00	7.45
ATOM	2682	O	TYR	609	64.448	24.514	88.207	1.00	10.10
ATOM	2683	N	HIS	610	62.803	23.416	87.137	1.00	4.17
ATOM	2684	CA	HIS	610	63.536	23.308	85.886	1.00	3.51
ATOM	2685	CB	HIS	610	64.306	21.995	85.775	1.00	2.85
ATOM	2686	CG	HIS	610	65.112	21.883	84.524	1.00	2.00
ATOM	2687	CD2	HIS	610	65.692	22.830	83.753	1.00	2.00
ATOM	2688	ND1	HIS	610	65.346	20.681	83.896	1.00	2.00
ATOM	2689	CE1	HIS	610	66.030	20.893	82.786	1.00	2.00
ATOM	2690	NE2	HIS	610	66.250	22.189	82.676	1.00	2.00
ATOM	2691	C	HIS	610	62.500	23.456	84.774	1.00	3.94
ATOM	2692	O	HIS	610	61.459	22.824	84.794	1.00	4.37
ATOM	2693	N	ARG	611	62.790	24.306	83.807	1.00	4.10
ATOM	2694	CA	ARG	611	61.858	24.561	82.756	1.00	2.00
ATOM	2695	CB	ARG	611	60.946	25.703	83.222	1.00	2.00
ATOM	2696	CG	ARG	611	59.476	25.573	82.826	1.00	5.34
ATOM	2697	CD	ARG	611	58.701	25.890	82.920	1.00	2.76
ATOM	2698	NE	ARG	611	57.501	26.833	82.093	1.00	4.99
ATOM	2699	CZ	ARG	611	56.647	27.834	81.931	1.00	4.31
ATOM	2700	NH1	ARG	611	56.850	28.973	82.542	1.00	9.07
ATOM	2701	NH2	ARG	611	55.605	27.711	81.138	1.00	2.00
ATOM	2702	C	ARG	611	62.657	24.994	81.558	1.00	2.00
ATOM	2703	O	ARG	611	63.800	25.350	81.680	1.00	3.11
ATOM	2704	N	VAL	612	62.074	24.833	80.388	1.00	2.76
ATOM	2705	CA	VAL	612	62.669	25.256	79.118	1.00	5.17
ATOM	2706	CB	VAL	612	63.056	24.068	78.198	1.00	5.26
ATOM	2707	CG1	VAL	612	63.806	24.567	76.967	1.00	6.96
ATOM	2708	CG2	VAL	612	63.917	23.089	78.935	1.00	9.67
ATOM	2709	C	VAL	612	61.490	25.968	73.464	1.00	4.40
ATOM	2710	O	VAL	612	60.382	25.436	78.481	1.00	5.97
ATOM	2711	N	ILE	613	61.674	27.187	77.968	1.00	2.39
ATOM	2712	CA	ILE	613	60.557	27.874	77.340	1.00	2.00
ATOM	2713	CB	ILE	613	59.889	28.933	78.270	1.00	2.00
ATOM	2714	CG2	ILE	613	59.244	28.279	79.471	1.00	2.16
ATOM	2715	CG1	ILE	613	60.890	30.015	73.669	1.00	2.00
ATOM	2716	CD1	ILE	613	60.267	31.241	79.182	1.00	2.00
ATOM	2717	C	ILE	613	60.996	28.601	76.094	1.00	3.35
ATOM	2718	O	ILE	613	62.164	28.553	75.709	1.00	2.06
ATOM	2719	N	HIS	614	60.012	29.173	75.412	1.00	3.35
ATOM	2720	CA	HIS	614	60.252	30.007	74.241	1.00	4.63
ATOM	2721	CB	HIS	614	59.604	29.427	72.970	1.00	2.35
ATOM	2722	CC	HIS	614	60.447	28.410	72.271	1.00	2.10

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ATOM	2723	CD2	HIS	614	61.353 28.536 71.281 1.00 2.96 4
ATOM	2724	ND1	HIS	614	60.442 27.075 72.609 1.00 4.63 7
ATOM	2725	CE1	HIS	614	61.310 26.419 71.865 1.00 2.00 5
ATOM	2726	NE2	HIS	614	61.875 27.284 71.051 1.00 6.31 7
ATOM	2727	C	HIS	614	59.580 31.311 74.664 1.00 3.58 5
ATOM	2728	C	HIS	614	58.419 31.306 75.046 1.00 2.50 3
ATOM	2729	N	ILE	615	60.315 32.412 74.674 1.00 2.76 7
ATOM	2730	CA	ILE	615	59.717 33.661 75.108 1.00 2.55 5
ATOM	2731	CB	ILE	615	60.770 34.768 75.221 1.00 2.49 5
ATOM	2732	CG2	ILE	615	60.102 36.115 75.307 1.00 2.99 5
ATOM	2733	CG1	ILE	615	61.785 34.387 76.307 1.00 2.00 6
ATOM	2734	CD1	ILE	615	63.067 35.246 76.351 1.00 2.00 5
ATOM	2735	C	ILE	615	58.569 34.079 74.205 1.00 3.27 5
ATOM	2736	O	ILE	615	57.609 34.687 74.651 1.00 5.04 3
ATOM	2737	N	ASN	616	58.639 33.673 72.943 1.00 5.73 7
ATOM	2738	CA	ASN	616	57.618 34.015 71.945 1.00 4.76 5
ATOM	2739	CB	ASN	616	58.205 33.893 70.513 1.00 2.00 6
ATOM	2740	CG	ASN	616	58.860 32.539 70.236 1.00 2.00 6
ATOM	2741	OD1	ASN	616	56.410 31.767 69.399 1.00 2.00 3
ATOM	2742	ND2	ASN	616	59.954 32.273 70.910 1.00 2.00 7
ATOM	2743	C	ASN	616	56.287 33.247 72.124 1.00 4.60 6
ATOM	2744	O	ASN	616	55.265 33.632 71.581 1.00 6.70 3
ATOM	2745	N	GLU	617	56.280 32.240 72.989 1.00 4.63 7
ATOM	2746	CA	GLU	617	55.088 31.444 73.242 1.00 5.16 6
ATOM	2747	CB	GLU	617	55.424 29.951 73.185 1.00 4.92 6
ATOM	2748	CG	GLU	617	56.381 29.633 72.086 1.00 8.53 5
ATOM	2749	CD	GLU	617	56.433 28.180 71.704 1.00 11.83 5
ATOM	2750	JE1	GLU	617	56.653 27.922 70.498 1.00 15.40 5
ATOM	2751	JE2	GLU	617	56.276 27.297 72.575 1.00 14.68 5
ATOM	2752	C	GLU	617	54.438 31.744 74.587 1.00 4.18 5
ATOM	2753	O	GLU	617	53.440 31.127 74.930 1.00 7.74 6
ATOM	2754	N	VAL	618	54.995 32.667 75.354 1.00 3.63 7
ATOM	2755	CA	VAL	618	54.433 32.988 76.655 1.00 2.00 6
ATOM	2756	CB	VAL	618	55.365 32.566 77.870 1.00 2.00 6
ATOM	2757	CG1	VAL	618	55.666 31.109 77.838 1.00 2.00 6
ATOM	2758	CG2	VAL	618	56.651 33.337 77.890 1.00 2.00 6
ATOM	2759	C	VAL	618	54.119 34.459 76.727 1.00 2.00 6
ATOM	2760	O	VAL	618	54.600 35.167 77.616 1.00 2.77 5
ATOM	2761	N	VAL	619	53.333 34.937 75.778 1.00 2.00 7
ATOM	2762	CA	VAL	619	52.970 36.345 75.792 1.00 3.10 6
ATOM	2763	CB	VAL	619	52.765 36.886 74.407 1.00 2.32 5
ATOM	2764	CG1	VAL	619	52.741 38.409 74.449 1.00 2.43 5
ATOM	2765	CG2	VAL	619	53.884 36.412 73.519 1.00 7.61 6
ATOM	2766	C	VAL	619	51.700 36.587 76.589 1.00 4.11 5
ATOM	2767	O	VAL	619	50.817 35.731 76.610 1.00 6.41 3
ATOM	2768	N	LEU	620	51.639 37.734 77.268 1.00 2.53 7
ATOM	2769	CA	LEU	620	50.492 38.143 78.080 1.00 3.37 5
ATOM	2770	CB	LEU	620	50.702 37.790 79.554 1.00 3.39 5
ATOM	2771	CG	LEU	620	49.612 37.183 80.438 1.00 3.95 6
ATOM	2772	CD1	LEU	620	50.233 37.141 81.775 1.00 5.62 5
ATOM	2773	CD2	LEU	620	48.306 37.985 80.529 1.00 3.31 5
ATOM	2774	C	LEU	620	50.382 39.654 77.920 1.00 5.44 5
ATOM	2775	O	LEU	620	50.656 40.437 78.736 1.00 7.07 8
ATOM	2776	N	LEU	621	49.739 40.044 76.834 1.00 7.07 7
ATOM	2777	CA	LEU	621	49.549 41.432 76.465 1.00 5.70 6
ATOM	2778	CB	LEU	621	48.832 41.498 75.111 1.00 5.58 6
ATOM	2779	CG	LEU	621	49.469 40.971 73.845 1.00 2.00 5
ATOM	2780	CD1	LEU	621	48.395 40.832 72.831 1.00 2.42 6
ATOM	2781	CD2	LEU	621	50.545 41.903 73.377 1.00 2.00 6
ATOM	2782	C	LEU	621	48.730 42.253 77.427 1.00 7.59 5
ATOM	2783	O	LEU	621	47.941 41.728 78.198 1.00 8.04 5
ATOM	2784	N	ASP	622	48.926 42.565 77.355 1.00 11.43 7
ATOM	2785	CA	ASP	622	48.148 44.513 78.128 1.00 10.55 5
ATOM	2786	CB	ASP	622	48.678 45.938 77.968 1.00 9.98 6
ATOM	2787	CG	ASP	622	49.746 46.300 78.963 1.00 11.16 5
ATOM	2788	CD1	ASP	622	50.398 47.342 78.724 1.00 12.42 5
ATOM	2789	CD2	ASP	622	49.927 45.580 79.976 1.00 11.12 5
ATOM	2790	C	ASP	622	46.855 44.429 77.336 1.00 10.98 5
ATOM	2791	O	ASP	622	46.867 44.075 76.152 1.00 11.16 3
ATOM	2792	N	ALA	623	45.754 44.808 77.965 1.00 13.11 7
ATOM	2793	CA	ALA	623	44.452 44.764 77.326 1.00 12.49 5
ATOM	2794	CB	ALA	623	43.375 44.723 78.402 1.00 13.24 5
ATOM	2795	C	ALA	623	44.267 45.975 76.399 1.00 10.77 5
ATOM	2796	O	ALA	623	45.013 46.953 76.489 1.00 11.45 3
ATOM	2797	N	PRO	624	43.311 45.890 75.462 1.00 7.62 7
ATOM	2798	CD	PRO	624	42.607 44.628 75.175 1.00 7.09 5
ATOM	2799	CA	PRO	624	42.969 46.928 74.486 1.00 6.69 5
ATOM	2800	CB	PRO	624	41.933 46.241 73.632 1.00 6.32 5



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ATOM	2801	CG PRO 624	42.334	44.750	73.736	1.00	9.96	5
ATOM	2802	C PRO 624	42.366	48.198	75.095	1.00	10.98	5
ATOM	2803	O PRO 624	41.591	48.139	76.056	1.00	13.90	5
ATOM	2804	N VAL 625	42.693	49.352	74.518	1.00	11.27	5
ATOM	2805	CA VAL 625	42.152	50.638	74.969	1.00	8.57	5
ATOM	2806	CB VAL 625	43.254	51.676	75.160	1.00	8.17	5
ATOM	2807	CG1 VAL 625	44.097	51.324	76.386	1.00	10.17	5
ATOM	2808	CG2 VAL 625	44.116	51.744	73.933	1.00	6.41	5
ATOM	2809	C VAL 625	41.136	51.193	73.950	1.00	11.00	5
ATOM	2810	O VAL 625	40.779	50.513	72.970	1.00	11.25	5
ATOM	2811	N GLY 626	40.629	52.392	74.243	1.00	10.53	7
ATOM	2812	CA GLY 626	39.683	53.098	73.389	1.00	12.11	5
ATOM	2813	C GLY 626	38.396	52.482	72.843	1.00	14.18	5
ATOM	2814	O GLY 626	37.906	52.907	71.775	1.00	14.32	3
ATOM	2815	N LEU 627	37.819	51.522	73.565	1.00	16.06	7
ATOM	2816	CA LEU 627	36.576	50.879	73.112	1.00	17.03	5
ATOM	2817	CB LEU 627	36.138	49.789	74.092	1.00	13.89	5
ATOM	2818	CG LEU 627	34.946	48.955	73.631	1.00	13.26	5
ATOM	2819	CD1 LEU 627	35.399	48.124	72.467	1.00	15.73	5
ATOM	2820	CD2 LEU 627	34.421	48.034	74.740	1.00	12.93	6
ATOM	2821	C LEU 627	35.415	51.869	72.928	1.00	18.27	5
ATOM	2822	O LEU 627	35.007	52.548	73.881	1.00	17.62	3
ATOM	2823	N VAL 628	34.954	52.005	71.682	1.00	19.54	7
ATOM	2824	CA VAL 628	33.814	52.862	71.355	1.00	19.76	5
ATOM	2825	CB VAL 628	34.166	54.119	70.490	1.00	18.01	5
ATOM	2826	CG1 VAL 628	34.935	55.151	71.318	1.00	19.05	5
ATOM	2827	CG2 VAL 628	34.942	53.723	69.244	1.00	18.46	5
ATOM	2828	C VAL 628	32.787	52.009	70.609	1.00	21.07	5
ATOM	2829	O VAL 628	33.146	51.171	69.740	1.00	19.35	3
ATOM	2830	N ALA 629	31.528	52.157	71.036	1.00	21.23	7
ATOM	2831	CA ALA 629	30.393	51.453	70.440	1.00	21.69	5
ATOM	2832	CB ALA 629	29.532	50.850	71.531	1.00	25.97	5
ATOM	2833	C ALA 629	29.593	52.496	69.664	1.00	22.67	5
ATOM	2834	O ALA 629	29.684	53.693	69.980	1.00	23.69	8
ATOM	2835	N ARG 630	28.823	52.061	68.659	1.00	22.36	7
ATOM	2836	CA ARG 630	28.014	52.979	67.845	1.00	19.90	5
ATOM	2837	CB ARG 630	28.873	53.703	66.809	1.00	19.83	6
ATOM	2838	CG ARG 630	29.087	55.154	67.175	1.00	22.67	5
ATOM	2839	CD ARG 630	29.565	56.016	65.999	1.00	24.86	5
ATOM	2840	NE ARG 630	29.366	57.461	66.223	1.00	26.19	7
ATOM	2841	CZ ARG 630	29.627	58.112	67.368	1.00	28.04	5
ATOM	2842	NH1 ARG 630	30.108	57.460	68.455	1.00	26.78	7
ATOM	2843	NH2 ARG 630	29.421	59.440	67.426	1.00	26.78	7
ATOM	2844	C ARG 630	26.867	52.308	67.125	1.00	19.38	5
ATOM	2845	O ARG 630	26.945	51.133	66.744	1.00	19.93	3
ATOM	2846	N LEU 631	25.787	53.049	66.944	1.00	18.71	7
ATOM	2847	CA LEU 631	24.650	52.498	66.238	1.00	18.38	5
ATOM	2848	CB LEU 631	23.379	53.267	66.603	1.00	18.29	5
ATOM	2849	CG LEU 631	22.269	52.408	67.214	1.00	17.34	5
ATOM	2850	CD1 LEU 631	22.275	50.967	66.711	1.00	18.01	5
ATOM	2851	CD2 LEU 631	22.351	52.322	68.740	1.00	18.08	5
ATOM	2852	C LEU 631	24.826	52.770	64.791	1.00	21.02	5
ATOM	2853	O LEU 631	24.739	53.915	64.341	1.00	23.22	3
ATOM	2854	N ALA 632	25.094	51.758	64.057	1.00	21.42	7
ATOM	2855	CA ALA 632	25.170	51.975	62.641	1.00	22.08	5
ATOM	2856	CB ALA 632	25.601	50.699	61.943	1.00	23.97	5
ATOM	2857	C ALA 632	23.771	52.420	62.235	1.00	24.54	5
ATOM	2858	O ALA 632	22.964	51.604	61.790	1.00	25.46	8
ATOM	2859	N ASP 633	23.542	53.700	62.434	1.00	90.00	7
ATOM	2860	CA ASP 633	22.239	54.366	62.209	1.00	90.00	5
ATOM	2861	CB ASP 633	22.438	55.880	62.013	1.00	90.00	5
ATOM	2862	CG ASP 633	22.352	56.775	63.273	1.00	90.00	5
ATOM	2863	CD1 ASP 633	21.778	56.363	64.247	1.00	90.00	3
ATOM	2864	CD2 ASP 633	22.852	57.977	63.227	1.00	90.00	3
ATOM	2865	C ASP 633	21.466	53.894	60.931	1.00	90.00	5
ATOM	2866	O ASP 633	20.252	53.666	60.947	1.00	90.00	3
ATOM	2867	N GLU 634	22.137	53.747	59.792	1.00	90.00	7
ATOM	2868	CA GLU 634	21.428	53.465	58.504	1.00	90.00	5
ATOM	2869	CB GLU 634	22.349	53.756	57.325	1.00	90.00	5
ATOM	2870	CG GLU 634	22.847	55.203	57.327	1.00	90.00	5
ATOM	2871	CD GLU 634	23.766	55.525	56.150	1.00	90.00	5
ATOM	2872	OE1 GLU 634	24.012	54.625	55.250	1.00	90.00	3
ATOM	2873	OE2 GLU 634	24.295	56.697	56.049	1.00	90.00	3
ATOM	2874	C GLU 634	20.911	52.021	58.273	1.00	90.00	5
ATOM	2875	O GLU 634	20.024	51.726	57.553	1.00	90.00	3
ATOM	2876	N SER 635	21.465	51.135	59.165	1.00	90.00	7
ATOM	2877	CA SER 635	21.062	49.720	59.145	1.00	90.00	5
ATOM	2878	CB SER 635	22.288	48.820	56.394	1.00	90.00	5

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ATOM	2879	OG	SER	635	23.189	49.037	60.063	1.00	90.00	3	
ATOM	2880	C	SER	635	20.328	49.370	60.435	1.00	90.00	5	
ATOM	2881	O	SER	635	19.394	48.552	60.427	1.00	90.00	3	
ATOM	2882	N	GLY	636	20.780	50.010	61.468	1.00	90.00	7	
ATOM	2883	CA	GLY	636	20.217	49.834	62.821	1.00	90.00	5	
ATOM	2884	C	GLY	636	20.996	48.771	63.586	1.00	90.00	5	
ATOM	2885	O	GLY	636	20.541	47.640	63.790	1.00	90.00	5	
ATOM	2886	N	HIS	637	22.203	49.107	64.010	1.00	29.39	7	
ATOM	2887	CA	HIS	637	22.920	48.155	64.847	1.00	28.30	5	
ATOM	2888	CB	HIS	637	23.190	46.817	64.148	1.00	27.49	5	
ATOM	2889	CG	HIS	637	23.915	46.854	62.796	1.00	26.32	5	
ATOM	2890	CD2	HIS	637	25.124	47.337	62.400	1.00	26.14	5	
ATOM	2891	ND1	HIS	637	23.338	46.289	61.665	1.00	26.56	7	
ATOM	2892	CE1	HIS	637	24.176	46.428	60.659	1.00	26.93	5	
ATOM	2893	NE2	HIS	637	25.247	47.050	61.079	1.00	26.35	7	
ATOM	2894	C	HIS	637	24.223	48.651	65.427	1.00	27.39	6	
ATOM	2895	O	HIS	637	24.505	49.862	65.452	1.00	27.46	3	
ATOM	2896	N	VAL	638	24.921	47.631	65.868	1.00	25.98	7	
ATOM	2897	CA	VAL	638	26.119	47.770	66.646	1.00	22.67	5	
ATOM	2898	CB	VAL	638	26.169	46.693	67.730	1.00	23.93	5	
ATOM	2899	CG1	VAL	638	26.966	47.127	68.963	1.00	24.68	5	
ATOM	2900	CG2	VAL	638	24.781	46.310	68.251	1.00	23.20	5	
ATOM	2901	C	VAL	638	27.422	47.694	65.877	1.00	21.16	5	
ATOM	2902	O	VAL	638	27.763	46.687	65.236	1.00	17.80	3	
ATOM	2903	N	VAL	639	28.129	48.808	65.940	1.00	19.71	7	
ATOM	2904	CA	VAL	639	29.417	48.927	65.309	1.00	21.49	5	
ATOM	2905	CB	VAL	639	29.362	49.967	64.127	1.00	22.97	5	
ATOM	2906	CG1	VAL	639	30.383	51.140	64.296	1.00	22.32	5	
ATOM	2907	CG2	VAL	639	29.531	49.189	62.796	1.00	21.09	5	
ATOM	2908	C	VAL	639	30.503	49.131	66.402	1.00	18.72	5	
ATOM	2909	O	VAL	639	30.569	50.164	67.103	1.00	15.61	3	
ATOM	2910	N	LEU	640	31.245	48.035	66.588	1.00	17.29	7	
ATOM	2911	CA	LEU	640	32.312	47.853	67.567	1.00	15.07	6	
ATOM	2912	CB	LEU	640	32.296	46.385	68.002	1.00	11.06	5	
ATOM	2913	CG	LEU	640	31.948	45.925	69.398	1.00	9.33	6	
ATOM	2914	CD1	LEU	640	30.755	46.635	69.940	1.00	6.96	5	
ATOM	2915	CD2	LEU	640	31.703	44.456	69.328	1.00	7.60	5	
ATOM	2916	C	LEU	640	33.727	48.158	67.106	1.00	15.19	5	
ATOM	2917	O	LEU	640	34.319	47.345	66.393	1.00	13.52	3	
ATOM	2918	N	ARG	641	34.320	49.236	67.616	1.00	16.40	7	
ATOM	2919	CA	ARG	641	35.717	49.564	67.269	1.00	18.02	5	
ATOM	2920	CB	ARG	641	35.744	50.820	66.406	1.00	18.96	5	
ATOM	2921	CG	ARG	641	36.505	50.608	65.100	1.00	23.80	5	
ATOM	2922	CD	ARG	641	35.742	51.114	63.884	1.00	25.92	5	
ATOM	2923	NE	ARG	641	34.649	50.212	63.502	1.00	26.12	7	
ATOM	2924	CZ	ARG	641	33.446	50.620	63.085	1.00	27.21	5	
ATOM	2925	NH1	ARG	641	33.173	51.935	63.013	1.00	24.02	7	
ATOM	2926	NH2	ARG	641	22.538	49.716	62.685	1.00	23.76	7	
ATOM	2927	C	ARG	641	36.638	49.707	68.527	1.00	17.87	5	
ATOM	2928	O	ARG	641	36.119	49.879	69.655	1.00	19.51	3	
ATOM	2929	N	TRP	642	37.972	49.398	68.366	1.00	16.84	7	
ATOM	2930	CA	TRP	642	38.925	49.723	69.515	1.00	14.61	5	
ATOM	2931	CB	TRP	642	38.765	48.534	70.453	1.00	13.71	5	
ATOM	2932	CG	TRP	642	39.106	47.243	69.819	1.00	9.75	5	
ATOM	2933	CD2	TRP	642	38.203	46.359	69.133	1.00	10.16	5	
ATOM	2934	CE2	TRP	642	38.926	45.195	68.814	1.00	10.08	5	
ATOM	2935	CE3	TRP	642	36.855	46.438	68.760	1.00	8.27	5	
ATOM	2936	CD1	TRP	642	40.304	46.612	69.860	1.00	7.42	5	
ATOM	2937	NE1	TRP	642	40.208	45.377	69.267	1.00	10.16	7	
ATOM	2938	CZ2	TRP	642	38.345	44.116	68.150	1.00	8.53	5	
ATOM	2939	CZ3	TRP	642	36.289	45.374	68.098	1.00	7.26	5	
ATOM	2940	CH2	TRP	642	37.035	44.225	67.803	1.00	7.13	5	
ATOM	2941	C	TRP	642	40.424	49.824	69.178	1.00	15.14	5	
ATOM	2942	O	TRP	642	40.798	49.704	68.006	1.00	17.51	3	
ATOM	2943	N	LEU	643	41.275	49.982	70.207	1.00	12.07	7	
ATOM	2944	CA	LEU	643	42.747	50.063	70.039	1.00	13.34	5	
ATOM	2945	CB	LEU	643	43.310	51.312	70.676	1.00	9.27	5	
ATOM	2946	CG	LEU	643	42.887	52.627	70.081	1.00	9.05	5	
ATOM	2947	CD1	LEU	643	43.784	53.715	70.583	1.00	7.00	3	
ATOM	2948	CD2	LEU	643	43.012	52.525	68.601	1.00	9.98	3	
ATOM	2949	C	LEU	643	43.508	48.891	70.662	1.00	15.42	5	
ATOM	2950	O	LEU	643	43.096	48.351	71.697	1.00	19.66	5	
ATOM	2951	N	PRO	644	44.645	48.493	70.059	1.00	15.98	7	
ATOM	2952	CD	PRO	644	45.206	49.056	68.817	1.00	15.21	5	
ATOM	2953	CA	PRO	644	45.481	47.381	70.556	1.00	14.66	5	
ATOM	2954	CB	PRO	644	46.485	47.175	69.412	1.00	15.17	5	
ATOM	2955	CG	PRO	644	46.642	48.573	68.867	1.00	15.08	5	
ATOM	2956	C	PRO	644	46.192	47.793	71.851	1.00	11.57	5	

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ATOM	2957	O PRO	644	46.148	48.978	72.209	1.00	12.33
ATOM	2958	N PRO	645	46.806	46.824	72.588	1.00	10.67
ATOM	2959	CD PRO	645	46.832	45.392	72.229	1.00	10.47
ATOM	2960	CA PRO	645	47.530	47.049	73.851	1.00	9.59
ATOM	2961	CB PRO	645	48.279	45.746	74.038	1.00	10.22
ATOM	2962	CG PRO	645	47.321	44.742	73.502	1.00	9.51
ATOM	2963	C PRO	645	48.475	48.178	73.572	1.00	9.51
ATOM	2964	O PRO	645	49.211	48.142	72.605	1.00	11.71
ATOM	2965	N PRO	646	48.433	49.229	74.375	1.00	9.63
ATOM	2966	CD PRO	646	47.682	49.431	75.618	1.00	9.62
ATOM	2967	CA PRO	646	49.334	50.350	74.105	1.00	9.90
ATOM	2968	CB PRO	646	49.004	51.345	75.217	1.00	9.95
ATOM	2969	CG PRO	646	47.619	50.941	75.674	1.00	11.92
ATOM	2970	C PRO	646	50.809	49.956	74.116	1.00	13.01
ATOM	2971	O PRO	646	51.204	48.918	74.679	1.00	14.24
ATOM	2972	N GLU	647	51.620	50.786	73.470	1.00	13.38
ATOM	2973	CA GLU	647	53.043	50.546	73.383	1.00	14.58
ATOM	2974	CB GLU	647	53.753	51.217	74.552	1.00	15.62
ATOM	2975	CG GLU	647	53.788	52.737	74.380	1.00	19.18
ATOM	2976	CD GLU	647	54.239	53.470	75.640	1.00	20.10
ATOM	2977	OE1 GLU	647	53.641	53.215	76.715	1.00	22.78
ATOM	2978	OE2 GLU	647	55.175	54.305	75.563	1.00	19.41
ATOM	2979	C GLU	647	53.485	49.082	73.218	1.00	14.37
ATOM	2980	O GLU	647	54.508	48.697	73.795	1.00	18.36
ATOM	2981	N THR	648	52.755	48.316	72.384	1.00	11.24
ATOM	2982	CA THR	648	53.029	46.899	72.062	1.00	9.00
ATOM	2983	CB THR	648	51.832	45.984	72.452	1.00	9.78
ATOM	2984	OG1 THR	648	51.552	46.119	73.852	1.00	10.70
ATOM	2985	CG2 THR	648	52.134	44.533	72.141	1.00	8.04
ATOM	2986	C THR	648	53.295	46.761	70.534	1.00	9.27
ATOM	2987	O THR	648	52.584	47.370	69.715	1.00	9.52
ATOM	2988	N PRO	649	54.320	45.968	70.137	1.00	7.20
ATOM	2989	CD PRO	649	55.333	45.245	70.941	1.00	6.54
ATOM	2990	CA PRO	649	54.610	45.819	68.713	1.00	6.88
ATOM	2991	CB PRO	649	56.106	45.495	68.711	1.00	5.46
ATOM	2992	CG PRO	649	56.233	44.592	69.879	1.00	3.39
ATOM	2993	C PRO	649	53.827	44.707	68.075	1.00	8.17
ATOM	2994	O PRO	649	52.957	44.106	68.705	1.00	9.10
ATOM	2995	N MET	650	54.224	44.406	66.838	1.00	9.01
ATOM	2996	CA MET	650	53.645	43.363	65.987	1.00	9.79
ATOM	2997	CB MET	650	54.158	41.969	66.370	1.00	8.66
ATOM	2998	CG MET	650	55.676	41.834	66.230	1.00	7.85
ATOM	2999	SD MET	650	56.219	41.811	64.535	1.00	7.28
ATOM	3000	CE MET	650	56.577	40.141	64.037	1.00	2.00
ATOM	3001	C MET	650	52.112	43.354	65.975	1.00	11.50
ATOM	3002	O MET	650	51.478	42.289	65.991	1.00	13.41
ATOM	3003	N THR	651	51.581	44.546	65.891	1.00	11.63
ATOM	3004	CA THR	651	50.136	44.808	65.906	1.00	12.15
ATOM	3005	CB THR	651	49.858	46.198	65.323	1.00	13.04
ATOM	3006	OG1 THR	651	50.419	47.197	66.162	1.00	14.67
ATOM	3007	CG2 THR	651	48.364	46.502	65.187	1.00	15.74
ATOM	3008	C THR	651	49.353	43.784	65.039	1.00	12.51
ATOM	3009	O THR	651	48.309	43.264	65.454	1.00	16.75
ATOM	3010	N SER	652	49.866	43.478	63.829	1.00	11.13
ATOM	3011	CA SER	652	49.110	42.623	62.863	1.00	6.89
ATOM	3012	CB SER	652	49.510	42.949	61.416	1.00	5.16
ATOM	3013	OG SER	652	50.405	41.990	60.895	1.00	4.04
ATOM	3014	C SER	652	49.235	41.114	63.151	1.00	7.54
ATOM	3015	O SER	652	49.034	40.261	62.274	1.00	9.34
ATOM	3016	N HIS	653	49.523	40.795	64.390	1.00	7.77
ATOM	3017	CA HIS	653	49.584	39.399	64.805	1.00	6.49
ATOM	3018	CB HIS	653	50.991	39.071	65.253	1.00	6.61
ATOM	3019	CG HIS	653	51.892	38.953	64.029	1.00	9.79
ATOM	3020	CD2 HIS	653	52.285	37.884	63.288	1.00	9.28
ATOM	3021	ND1 HIS	653	52.471	40.071	63.438	1.00	10.33
ATOM	3022	CE1 HIS	653	53.171	39.668	62.395	1.00	5.42
ATOM	3023	NE2 HIS	653	53.071	38.367	62.291	1.00	7.91
ATOM	3024	C HIS	653	48.476	39.163	65.830	1.00	4.62
ATOM	3025	O HIS	653	47.989	38.044	65.994	1.00	5.90
ATOM	3026	N ILE	654	48.046	40.234	66.470	1.00	5.21
ATOM	3027	CA ILE	654	47.072	40.145	67.580	1.00	4.75
ATOM	3028	CB ILE	654	47.059	41.456	68.355	1.00	3.95
ATOM	3029	CG2 ILE	654	46.252	41.368	69.653	1.00	5.93
ATOM	3030	CG1 ILE	654	48.469	41.891	68.760	1.00	3.24
ATOM	3031	CD1 ILE	654	48.560	43.367	69.131	1.00	2.00
ATOM	3032	C ILE	654	45.633	39.787	67.156	1.00	5.10
ATOM	3033	O ILE	654	44.981	40.508	66.395	1.00	7.39
ATOM	3034	N ARG	655	45.214	38.661	67.713	1.00	5.70

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ATOM	3035	CA	ARG	655	43.856	38.107	67.582	1.00	4.70	5
ATOM	3036	CB	ARG	655	43.947	36.608	67.851	1.00	6.54	6
ATOM	3037	CG	ARG	655	42.732	35.835	67.393	1.00	12.78	5
ATOM	3038	CD	ARG	655	42.923	35.234	66.013	1.00	19.16	5
ATOM	3039	NE	ARG	655	41.690	35.243	65.243	1.00	25.22	7
ATOM	3040	CZ	ARG	655	41.487	34.509	64.155	1.00	28.18	5
ATOM	3041	NH1	ARG	655	42.441	33.699	63.683	1.00	29.93	7
ATOM	3042	NH2	ARG	655	40.343	34.523	63.465	1.00	30.11	7
ATOM	3043	C	ARG	655	43.012	38.786	68.687	1.00	4.93	6
ATOM	3044	O	ARG	655	43.561	39.225	69.706	1.00	4.78	9
ATOM	3045	N	TYR	656	41.706	38.916	68.485	1.00	3.05	7
ATOM	3046	CA	TYR	656	40.852	39.533	69.491	1.00	4.57	6
ATOM	3047	CB	TYR	656	40.315	40.886	69.041	1.00	5.74	6
ATOM	3048	CG	TYR	656	41.339	41.973	69.131	1.00	11.08	5
ATOM	3049	CD1	TYR	656	41.994	42.423	67.995	1.00	11.86	6
ATOM	3050	CE1	TYR	656	43.029	43.341	68.077	1.00	13.79	6
ATOM	3051	CD2	TYR	656	41.736	42.482	70.366	1.00	13.83	6
ATOM	3052	CE2	TYR	656	42.779	43.407	70.461	1.00	14.75	6
ATOM	3053	CZ	TYR	656	43.422	43.826	69.307	1.00	14.26	6
ATOM	3054	OH	TYR	656	44.498	44.701	69.373	1.00	19.33	8
ATOM	3055	C	TYR	656	39.693	38.646	69.848	1.00	7.31	5
ATOM	3056	O	TYR	656	39.504	37.608	69.210	1.00	7.58	8
ATOM	3057	N	GLU	657	38.967	39.048	70.905	1.00	9.63	7
ATOM	3058	CA	GLU	657	37.776	38.359	71.431	1.00	9.06	5
ATOM	3059	CB	GLU	657	38.109	37.385	72.555	1.00	11.39	6
ATOM	3060	CG	GLU	657	36.874	36.766	73.217	1.00	14.76	6
ATOM	3061	CD	GLU	657	36.755	35.254	72.977	1.00	17.29	6
ATOM	3062	OE1	GLU	657	36.157	34.838	71.945	1.00	19.32	2
ATOM	3063	OE2	GLU	657	37.245	34.472	73.826	1.00	18.57	8
ATOM	3064	C	GLU	657	36.827	39.366	72.006	1.00	10.04	6
ATOM	3065	O	GLU	657	37.163	40.033	72.985	1.00	8.78	8
ATOM	3066	N	VAL	658	35.635	39.428	71.412	1.00	13.32	7
ATOM	3067	CA	VAL	658	34.550	40.334	71.819	1.00	15.04	6
ATOM	3068	CB	VAL	658	33.826	40.908	70.578	1.00	17.13	6
ATOM	3069	CG1	VAL	658	32.355	41.228	70.903	1.00	18.15	6
ATOM	3070	CG2	VAL	658	34.552	42.151	70.055	1.00	15.29	6
ATOM	3071	C	VAL	658	33.518	39.602	72.697	1.00	15.57	6
ATOM	3072	O	VAL	658	33.025	38.519	72.336	1.00	16.39	8
ATOM	3073	N	ASP	659	33.168	40.225	73.818	1.00	15.80	7
ATOM	3074	CA	ASP	659	32.217	39.660	74.762	1.00	16.22	6
ATOM	3075	CB	ASP	659	32.857	39.583	76.152	1.00	18.33	6
ATOM	3076	CG	ASP	659	31.841	39.320	77.262	1.00	17.02	6
ATOM	3077	OD1	ASP	659	31.706	40.220	78.127	1.00	16.96	8
ATOM	3078	OD2	ASP	659	31.191	38.238	77.248	1.00	15.05	8
ATOM	3079	C	ASP	659	30.959	40.488	74.877	1.00	17.09	6
ATOM	3080	O	ASP	659	30.946	41.480	75.641	1.00	16.55	3
ATOM	3081	N	VAL	660	29.924	40.096	74.127	1.00	17.40	7
ATOM	3082	CA	VAL	660	28.623	40.775	74.150	1.00	18.10	5
ATOM	3083	CB	VAL	660	27.835	40.550	72.857	1.00	15.37	5
ATOM	3084	CG1	VAL	660	28.760	40.397	71.683	1.00	16.34	5
ATOM	3085	CG2	VAL	660	26.931	39.368	72.990	1.00	15.04	5
ATOM	3086	C	VAL	660	27.768	40.299	75.335	1.00	20.40	5
ATOM	3087	O	VAL	660	27.719	39.092	75.655	1.00	21.69	8
ATOM	3088	N	SER	661	27.018	41.218	75.943	1.00	22.33	7
ATOM	3089	CA	SER	661	26.210	40.865	77.104	1.00	23.37	6
ATOM	3090	CB	SER	661	27.146	40.683	78.308	1.00	23.56	6
ATOM	3091	OG	SER	661	28.007	39.569	78.169	1.00	25.08	8
ATOM	3092	C	SER	661	25.132	41.882	77.544	1.00	23.29	6
ATOM	3093	O	SER	661	24.814	42.901	76.839	1.00	24.57	8
ATOM	3094	N	ALA	662	24.676	41.596	78.784	1.00	26.02	7
ATOM	3095	CA	ALA	662	23.690	42.325	79.598	1.00	23.48	5
ATOM	3096	CB	ALA	662	23.909	43.856	79.493	1.00	24.66	5
ATOM	3097	C	ALA	662	22.242	41.933	79.339	1.00	22.08	5
ATOM	3098	O	ALA	662	21.935	40.739	79.266	1.00	16.69	8
ATOM	3099	N	GLY	663	21.367	42.948	79.300	1.00	23.15	7
ATOM	3100	CA	GLY	663	19.936	42.775	79.047	1.00	24.87	5
ATOM	3101	C	GLY	663	19.124	41.953	80.038	1.00	23.53	5
ATOM	3102	O	GLY	663	18.542	40.929	79.649	1.00	22.72	8
ATOM	3103	N	ASN	664	19.032	42.452	81.277	1.00	24.09	7
ATOM	3104	CA	ASN	664	18.317	41.816	82.410	1.00	25.56	5
ATOM	3105	CE	ASN	664	17.157	42.706	82.938	1.00	27.33	5
ATOM	3106	CG	ASN	664	15.907	42.725	82.013	1.00	28.05	5
ATOM	3107	OD1	ASN	664	15.791	43.575	81.114	1.00	29.36	8
ATOM	3108	ND2	ASN	664	14.939	41.852	82.294	1.00	26.86	7
ATOM	3109	C	ASN	664	17.831	40.352	82.334	1.00	25.76	5
ATOM	3110	O	ASN	664	16.976	39.992	81.488	1.00	25.92	8
ATOM	3111	N	GLY	665	18.250	39.517	82.243	1.00	24.45	7
ATOM	3112	CA	GLY	665	17.918	38.123	82.294	1.00	24.29	5

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ATOM	3113	C	GLY	665	18.560	37.239	82.235	1.00	23.94	5
ATOM	3114	O	GLY	665	18.754	36.011	82.454	1.00	24.01	5
ATOM	3115	N	ALA	666	18.767	37.805	81.047	1.00	22.31	7
ATOM	3116	CA	ALA	666	19.457	37.054	80.035	1.00	22.71	5
ATOM	3117	CB	ALA	666	19.331	37.724	78.693	1.00	21.95	5
ATOM	3118	C	ALA	666	20.893	37.166	80.577	1.00	24.38	5
ATOM	3119	O	ALA	666	21.300	38.225	81.075	1.00	25.18	8
ATOM	3120	N	GLY	667	21.579	36.036	80.672	1.00	25.52	7
ATOM	3121	CA	GLY	667	22.941	36.058	81.159	1.00	26.48	5
ATOM	3122	C	GLY	667	23.838	35.946	79.949	1.00	28.11	5
ATOM	3123	O	GLY	667	24.789	35.145	79.937	1.00	29.47	5
ATOM	3124	N	SER	668	23.483	36.689	78.896	1.00	28.73	7
ATOM	3125	CA	SER	668	24.256	36.669	77.641	1.00	28.04	6
ATOM	3126	CB	SER	668	23.634	37.605	76.547	1.00	28.80	5
ATOM	3127	OG	SER	668	24.312	37.574	75.278	1.00	24.54	8
ATOM	3128	C	SER	668	25.597	37.209	78.057	1.00	27.60	6
ATOM	3129	O	SER	668	25.647	38.220	78.798	1.00	27.37	8
ATOM	3130	N	VAL	669	26.623	36.397	77.762	1.00	26.59	7
ATOM	3131	CA	VAL	669	28.049	36.715	77.987	1.00	23.08	6
ATOM	3132	CB	VAL	669	28.665	35.974	79.266	1.00	20.59	6
ATOM	3133	CG1	VAL	669	28.460	34.484	79.178	1.00	19.42	5
ATOM	3134	CG2	VAL	669	30.175	36.316	79.456	1.00	20.06	6
ATOM	3135	C	VAL	669	28.668	36.266	76.644	1.00	21.55	5
ATOM	3136	O	VAL	669	29.846	35.888	76.545	1.00	20.19	8
ATOM	3137	N	GLN	670	27.845	36.409	75.598	1.00	20.21	7
ATOM	3138	CA	GLN	670	28.193	36.009	74.245	1.00	18.75	6
ATOM	3139	CB	GLN	670	27.005	36.236	73.312	1.00	17.59	6
ATOM	3140	CG	GLN	670	27.182	35.569	71.935	1.00	22.13	6
ATOM	3141	CD	GLN	670	27.933	36.432	70.902	1.00	22.70	6
ATOM	3142	OE1	GLN	670	28.500	37.485	71.234	1.00	24.66	8
ATOM	3143	NE2	GLN	670	27.912	35.995	69.634	1.00	23.69	7
ATOM	3144	C	GLN	670	29.519	36.583	73.696	1.00	17.46	6
ATOM	3145	O	GLN	670	29.792	37.782	73.770	1.00	15.56	8
ATOM	3146	N	ARG	671	30.332	35.679	73.157	1.00	15.69	7
ATOM	3147	CA	ARG	671	31.631	36.013	72.639	1.00	16.60	6
ATOM	3148	CB	ARG	671	32.678	35.334	73.517	1.00	17.57	6
ATOM	3149	CG	ARG	671	32.946	36.061	74.887	1.00	19.96	6
ATOM	3150	CD	ARG	671	32.493	35.269	76.139	1.00	18.73	6
ATOM	3151	NE	ARG	671	32.986	35.894	77.368	1.00	19.78	7
ATOM	3152	CZ	ARG	671	33.863	35.344	78.218	1.00	19.40	6
ATOM	3153	NH1	ARG	671	34.370	34.124	78.021	1.00	17.08	7
ATOM	3154	NH2	ARG	671	34.304	36.062	79.241	1.00	17.95	7
ATOM	3155	C	ARG	671	31.869	35.669	71.158	1.00	18.54	6
ATOM	3156	O	ARG	671	31.425	34.618	70.645	1.00	20.62	8
ATOM	3157	N	VAL	672	32.576	36.556	70.460	1.00	18.18	7
ATOM	3158	CA	VAL	672	32.879	36.337	69.049	1.00	15.30	6
ATOM	3159	CB	VAL	672	32.079	37.317	68.160	1.00	15.97	5
ATOM	3160	CG1	VAL	672	30.649	37.440	68.682	1.00	17.58	5
ATOM	3161	CG2	VAL	672	32.728	38.702	68.133	1.00	17.86	6
ATOM	3162	C	VAL	672	34.379	36.538	68.849	1.00	14.22	6
ATOM	3163	O	VAL	672	34.964	37.495	69.358	1.00	14.18	8
ATOM	3164	N	GLU	673	35.011	35.587	68.184	1.00	13.30	7
ATOM	3165	CA	GLU	673	35.437	35.666	67.911	1.00	14.85	6
ATOM	3166	CB	GLU	673	36.902	34.409	67.150	1.00	17.98	6
ATOM	3167	CG	GLU	673	36.621	34.525	65.601	1.00	21.07	5
ATOM	3168	CD	GLU	673	36.996	33.299	64.759	1.00	22.50	5
ATOM	3169	OE1	GLU	673	36.964	32.153	63.300	1.00	20.19	8
ATOM	3170	OE2	GLU	673	37.279	33.501	63.537	1.00	23.59	8
ATOM	3171	C	GLU	673	36.645	36.859	66.978	1.00	14.79	5
ATOM	3172	O	GLU	673	35.688	37.420	66.456	1.00	15.66	8
ATOM	3173	N	ILE	674	37.899	37.192	66.708	1.00	15.73	7
ATOM	3174	CA	ILE	674	38.224	38.270	65.790	1.00	15.34	5
ATOM	3175	CB	ILE	674	38.340	39.659	66.498	1.00	16.72	5
ATOM	3176	CG2	ILE	674	38.785	40.718	65.483	1.00	15.50	5
ATOM	3177	CG1	ILE	674	37.060	40.044	67.289	1.00	15.11	5
ATOM	3178	CD1	ILE	674	35.824	40.386	66.489	1.00	12.07	5
ATOM	3179	C	ILE	674	39.596	37.922	65.198	1.00	16.94	5
ATOM	3180	O	ILE	674	40.511	37.502	65.909	1.00	15.56	3
ATOM	3181	N	LEU	675	39.722	38.012	63.884	1.00	18.65	7
ATOM	3182	CA	LEU	675	41.000	37.737	63.251	1.00	16.13	5
ATOM	3183	CB	LEU	675	40.846	37.553	61.744	1.00	16.02	5
ATOM	3184	CG	LEU	675	40.335	36.155	61.359	1.00	17.94	5
ATOM	3185	CD1	LEU	675	38.786	36.050	61.326	1.00	13.53	5
ATOM	3186	CD2	LEU	675	40.967	35.743	60.014	1.00	18.65	6
ATOM	3187	C	LEU	675	41.944	38.895	63.585	1.00	16.58	5
ATOM	3188	O	LEU	675	41.500	40.013	63.920	1.00	16.45	8
ATOM	3189	N	GLU	676	43.240	38.587	63.521	1.00	14.67	7
ATOM	3190	CA	GLU	676	44.316	39.514	63.829	1.00	12.70	5

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ATOM	3191	CB	GLU	676	45.667	38.907	63.526	1.00	12.08
ATOM	3192	CG	GLU	676	45.627	37.882	62.478	1.00	11.18
ATOM	3193	CD	GLU	676	45.494	36.518	63.080	1.00	13.77
ATOM	3194	OE1	GLU	676	46.538	36.007	63.546	1.00	16.32
ATOM	3195	OE2	GLU	676	44.367	35.967	63.108	1.00	13.00
ATOM	3196	C	GLU	676	44.268	40.836	63.146	1.00	12.13
ATOM	3197	O	GLU	676	43.569	41.007	62.159	1.00	12.89
ATOM	3198	N	GLY	677	45.030	41.772	63.699	1.00	11.52
ATOM	3199	CA	GLY	677	45.121	43.103	63.145	1.00	11.07
ATOM	3200	C	GLY	677	43.796	43.794	62.961	1.00	11.96
ATOM	3201	O	GLY	677	43.770	44.949	62.523	1.00	14.32
ATOM	3202	N	ARG	678	42.700	43.134	63.329	1.00	12.98
ATOM	3203	CA	ARG	678	41.387	43.743	63.174	1.00	14.43
ATOM	3204	CB	ARG	678	40.342	42.666	62.927	1.00	13.34
ATOM	3205	CG	ARG	678	39.529	42.932	61.695	1.00	15.05
ATOM	3206	CD	ARG	678	40.401	42.681	60.504	1.00	17.70
ATOM	3207	NE	ARG	678	41.014	41.368	60.643	1.00	22.61
ATOM	3208	CZ	ARG	678	41.887	40.845	59.787	1.00	23.28
ATOM	3209	NH1	ARG	678	42.274	41.525	58.700	1.00	22.06
ATOM	3210	NH2	ARG	678	42.380	39.631	60.037	1.00	25.26
ATOM	3211	C	ARG	678	41.001	44.532	64.420	1.00	14.43
ATOM	3212	O	ARG	678	41.199	44.034	63.529	1.00	15.07
ATOM	3213	N	THR	679	40.462	45.743	64.249	1.00	13.15
ATOM	3214	CA	THR	679	40.027	46.552	65.390	1.00	14.13
ATOM	3215	CB	THR	679	40.996	47.685	65.669	1.00	14.19
ATOM	3216	OG1	THR	679	41.204	48.405	64.448	1.00	17.57
ATOM	3217	CG2	THR	679	42.332	47.148	66.229	1.00	13.59
ATOM	3218	C	THR	679	38.637	47.171	65.182	1.00	16.43
ATOM	3219	O	THR	679	38.393	48.336	65.340	1.00	15.23
ATOM	3220	N	GLU	680	37.732	46.384	64.604	1.00	18.09
ATOM	3221	CA	GLU	680	36.358	46.812	64.332	1.00	19.04
ATOM	3222	CB	GLU	680	36.289	47.763	63.128	1.00	18.69
ATOM	3223	CG	GLU	680	36.140	47.101	61.755	1.00	18.32
ATOM	3224	CD	GLU	680	35.086	47.782	60.847	1.00	18.05
ATOM	3225	OE1	GLU	680	34.342	47.032	60.138	1.00	16.53
ATOM	3226	OE2	GLU	680	35.019	49.045	60.825	1.00	14.40
ATOM	3227	C	GLU	680	35.489	45.579	64.076	1.00	21.29
ATOM	3228	O	GLU	680	35.887	44.641	63.364	1.00	22.54
ATOM	3229	N	CYS	681	34.299	45.578	64.654	1.00	22.91
ATOM	3230	CA	CYS	681	33.382	44.462	64.498	1.00	24.61
ATOM	3231	CB	CYS	681	33.617	43.402	65.603	1.00	26.42
ATOM	3232	SG	CYS	681	32.134	42.836	66.606	1.00	26.71
ATOM	3233	C	CYS	681	31.958	45.006	64.540	1.00	24.30
ATOM	3234	O	CYS	681	31.579	45.763	65.448	1.00	23.84
ATOM	3235	N	VAL	682	31.181	44.688	63.517	1.00	21.58
ATOM	3236	CA	VAL	682	29.818	45.174	63.511	1.00	20.10
ATOM	3237	CB	VAL	682	29.433	45.877	62.131	1.00	18.07
ATOM	3238	CG1	VAL	682	30.190	45.270	60.969	1.00	16.40
ATOM	3239	CG2	VAL	682	27.952	45.785	61.867	1.00	17.19
ATOM	3240	C	VAL	682	28.861	44.077	64.001	1.00	17.00
ATOM	3241	O	VAL	682	28.659	43.049	63.342	1.00	15.10
ATOM	3242	N	LEU	683	28.449	44.218	65.258	1.00	17.47
ATOM	3243	CA	LEU	683	27.495	43.254	65.659	1.00	20.70
ATOM	3244	CB	LEU	683	27.326	43.584	67.348	1.00	17.50
ATOM	3245	CG	LEU	683	28.420	43.127	68.299	1.00	13.82
ATOM	3246	CD1	LEU	683	28.201	43.741	69.667	1.00	13.45
ATOM	3247	CD2	LEU	683	28.376	41.638	68.387	1.00	15.36
ATOM	3248	C	LEU	683	26.228	43.730	65.104	1.00	24.03
ATOM	3249	O	LEU	683	25.446	44.610	65.544	1.00	24.27
ATOM	3250	N	SER	684	26.087	43.161	63.914	1.00	25.99
ATOM	3251	CA	SER	684	25.003	43.521	63.028	1.00	26.98
ATOM	3252	CB	SER	684	25.222	42.906	61.629	1.00	31.20
ATOM	3253	OG	SER	684	26.502	43.257	61.067	1.00	36.99
ATOM	3254	C	SER	684	23.614	43.199	63.491	1.00	26.69
ATOM	3255	O	SER	684	22.800	44.106	63.699	1.00	27.76
ATOM	3256	N	ASN	685	23.397	41.945	63.826	1.00	24.94
ATOM	3257	CA	ASN	685	22.049	41.496	64.131	1.00	25.85
ATOM	3258	CB	ASN	685	21.716	40.428	63.083	1.00	27.66
ATOM	3259	CG	ASN	685	22.993	39.749	62.504	1.00	28.61
ATOM	3260	OD1	ASN	685	23.994	40.433	62.186	1.00	26.41
ATOM	3261	ND2	ASN	685	22.972	38.406	62.407	1.00	28.57
ATOM	3262	C	ASN	685	21.748	40.978	65.533	1.00	26.76
ATOM	3263	O	ASN	685	22.271	39.905	65.923	1.00	27.14
ATOM	3264	N	LEU	686	20.899	41.704	66.287	1.00	25.95
ATOM	3265	CA	LEU	686	20.583	41.260	67.649	1.00	24.26
ATOM	3266	CB	LEU	686	21.779	41.525	68.584	1.00	22.44
ATOM	3267	CG	LEU	686	22.718	42.760	68.474	1.00	23.47
ATOM	3268	CD1	LEU	686	23.700	42.846	69.708	1.00	21.84

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ATOM	3269	CD2	LEU	686	23.563	42.742	67.173	1.00	20.88	5
ATOM	3270	C	LEU	686	19.233	41.566	68.375	1.00	26.62	5
ATOM	3271	O	LEU	686	18.361	40.669	68.478	1.00	27.06	8
ATOM	3272	N	ARG	687	19.035	42.801	68.858	1.00	25.21	7
ATOM	3273	CA	ARG	687	17.838	43.147	69.636	1.00	21.90	5
ATOM	3274	CB	ARG	687	18.117	42.901	71.113	1.00	21.00	5
ATOM	3275	CG	ARG	687	17.254	41.847	71.745	1.00	18.87	5
ATOM	3276	CD	ARG	687	17.778	40.471	71.410	1.00	20.25	5
ATOM	3277	NE	ARG	687	16.883	39.426	71.911	1.00	23.57	7
ATOM	3278	CZ	ARG	687	16.832	38.188	71.416	1.00	24.78	5
ATOM	3279	NH1	ARG	687	17.636	37.837	70.405	1.00	25.89	7
ATOM	3280	NH2	ARG	687	15.969	37.303	71.908	1.00	23.14	7
ATOM	3281	C	ARG	687	17.358	44.587	69.517	1.00	23.37	5
ATOM	3282	O	ARG	687	17.863	45.369	68.695	1.00	24.06	8
ATOM	3283	N	GLY	688	16.420	44.939	70.407	1.00	23.79	7
ATOM	3284	CA	GLY	688	15.825	46.263	70.434	1.00	22.75	5
ATOM	3285	C	GLY	688	15.583	46.644	71.874	1.00	23.19	6
ATOM	3286	O	GLY	688	15.359	45.760	72.726	1.00	21.67	8
ATOM	3287	N	ARG	689	15.712	47.944	72.154	1.00	23.01	7
ATOM	3288	CA	ARG	689	15.531	48.533	73.500	1.00	23.70	6
ATOM	3289	CB	ARG	689	14.034	48.518	73.902	1.00	22.81	6
ATOM	3290	CG	ARG	689	13.543	49.819	74.581	1.00	20.45	5
ATOM	3291	CD	ARG	689	13.398	50.988	73.575	1.00	18.41	5
ATOM	3292	NE	ARG	689	14.071	52.266	73.908	1.00	17.79	7
ATOM	3293	CZ	ARG	689	14.201	52.828	73.128	1.00	19.24	5
ATOM	3294	NH1	ARG	689	13.738	52.253	76.250	1.00	12.88	7
ATOM	3295	NH2	ARG	689	14.704	54.066	75.213	1.00	18.71	7
ATOM	3296	C	ARG	689	16.425	47.958	74.648	1.00	25.87	5
ATOM	3297	O	ARG	689	16.512	48.542	75.756	1.00	25.28	8
ATOM	3298	N	THR	690	17.153	46.887	74.313	1.00	25.78	7
ATOM	3299	CA	THR	690	18.053	46.127	75.182	1.00	23.94	6
ATOM	3300	CB	THR	690	18.530	44.902	74.403	1.00	24.95	6
ATOM	3301	OG1	THR	690	17.550	44.550	73.405	1.00	24.96	8
ATOM	3302	CG2	THR	690	18.808	43.736	75.355	1.00	24.38	5
ATOM	3303	C	THR	690	19.337	46.821	75.661	1.00	27.33	6
ATOM	3304	O	THR	690	20.052	47.436	74.841	1.00	25.88	8
ATOM	3305	N	ARG	691	19.653	46.704	76.966	1.00	28.66	7
ATOM	3306	CA	ARG	691	20.920	47.275	77.514	1.00	27.60	6
ATOM	3307	CB	ARG	691	20.908	47.426	79.055	1.00	28.38	5
ATOM	3308	CG	ARG	691	21.668	46.303	79.860	1.00	30.17	5
ATOM	3309	CD	ARG	691	21.736	46.597	81.403	1.00	30.51	5
ATOM	3310	NE	ARG	691	22.360	45.549	82.240	1.00	29.33	7
ATOM	3311	CZ	ARG	691	21.681	44.632	82.957	1.00	31.23	5
ATOM	3312	NH1	ARG	691	20.331	44.612	82.931	1.00	32.13	7
ATOM	3313	NH2	ARG	691	22.337	43.775	83.768	1.00	28.34	7
ATOM	3314	C	ARG	691	22.024	46.269	77.114	1.00	27.87	5
ATOM	3315	O	ARG	691	21.863	45.028	77.231	1.00	28.65	8
ATOM	3316	N	TYR	692	23.157	46.781	76.682	1.00	27.18	7
ATOM	3317	CA	TYR	692	24.213	45.893	76.256	1.00	23.54	5
ATOM	3318	CB	TYR	692	24.237	45.885	74.744	1.00	24.61	5
ATOM	3319	CG	TYR	692	23.317	44.905	74.100	1.00	23.60	5
ATOM	3320	CD1	TYR	692	23.303	43.575	74.501	1.00	23.69	5
ATOM	3321	CE1	TYR	692	22.544	42.636	73.833	1.00	23.82	5
ATOM	3322	CD2	TYR	692	22.535	45.283	73.014	1.00	24.04	5
ATOM	3323	CE2	TYR	692	21.755	44.345	72.325	1.00	24.91	6
ATOM	3324	CZ	TYR	692	21.772	43.022	72.745	1.00	24.40	5
ATOM	3325	OH	TYR	692	21.021	42.086	72.059	1.00	27.00	8
ATOM	3326	C	TYR	692	25.534	46.436	76.739	1.00	22.44	6
ATOM	3327	O	TYR	692	25.776	47.643	76.606	1.00	21.10	8
ATOM	3328	N	THR	693	26.382	45.567	77.302	1.00	19.16	7
ATOM	3329	CA	THR	693	27.711	45.989	77.758	1.00	14.99	5
ATOM	3330	CB	THR	693	27.877	45.985	79.301	1.00	13.81	5
ATOM	3331	OG1	THR	693	26.746	46.642	79.909	1.00	14.05	8
ATOM	3332	CG2	THR	693	29.155	46.745	79.685	1.00	12.28	5
ATOM	3333	C	THR	693	28.733	45.070	77.062	1.00	14.45	5
ATOM	3334	O	THR	693	28.450	43.870	76.926	1.00	11.01	8
ATOM	3335	N	PHE	694	29.811	45.661	76.604	1.00	15.34	7
ATOM	3336	CA	PHE	694	30.841	44.969	75.845	1.00	15.68	5
ATOM	3337	CB	PHE	694	30.833	45.501	74.405	1.00	18.12	5
ATOM	3338	CG	PHE	694	29.457	45.682	73.816	1.00	19.49	5
ATOM	3339	CD1	PHE	694	28.740	46.860	74.043	1.00	18.66	6
ATOM	3340	CD2	PHE	694	28.882	44.679	73.015	1.00	18.42	5
ATOM	3341	CE1	PHE	694	27.480	47.035	73.481	1.00	19.71	5
ATOM	3342	CE2	PHE	694	27.617	44.854	72.450	1.00	16.44	6
ATOM	3343	CZ	PHE	694	26.919	46.024	72.679	1.00	16.79	5
ATOM	3344	C	PHE	694	32.237	45.210	76.374	1.00	14.83	6
ATOM	3345	O	PHE	694	32.533	46.304	76.835	1.00	14.75	8
ATOM	3346	N	ALA	695	33.112	44.227	76.155	1.00	14.22	7

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ATOM	3347	CA ALA	695	34.532	44.271	76.533	1.00	14.58 6
ATOM	3348	CB ALA	695	34.704	43.821	77.959	1.00	15.52 6
ATOM	3349	C ALA	695	35.331	43.352	75.579	1.00	16.59 6
ATOM	3350	O ALA	695	34.739	42.503	74.883	1.00	16.77 6
ATOM	3351	N VAL	696	36.663	43.475	75.554	1.00	18.89 7
ATOM	3352	CA VAL	696	37.475	42.637	74.640	1.00	18.54 6
ATOM	3353	CB VAL	696	37.455	43.242	73.198	1.00	19.19 6
ATOM	3354	CG1 VAL	696	37.867	44.705	73.223	1.00	17.15 6
ATOM	3355	CG2 VAL	696	38.335	42.446	72.255	1.00	20.60 6
ATOM	3356	C VAL	696	38.923	42.284	75.047	1.00	18.64 6
ATOM	3357	O VAL	696	39.654	43.093	75.637	1.00	18.43 6
ATOM	3358	N ARG	697	39.321	41.055	74.738	1.00	18.97 7
ATOM	3359	CA ARG	697	40.675	40.563	75.050	1.00	18.67 6
ATOM	3360	CB ARG	697	40.593	39.173	75.664	1.00	17.03 6
ATOM	3361	CG ARG	697	39.772	39.078	76.889	1.00	15.40 6
ATOM	3362	CD ARG	697	39.842	37.650	77.417	1.00	18.07 6
ATOM	3363	NE ARG	697	39.077	36.676	76.632	1.00	17.47 7
ATOM	3364	CZ ARG	697	38.722	35.467	77.081	1.00	19.24 6
ATOM	3365	NH1 ARG	697	39.061	35.078	78.309	1.00	20.70 7
ATOM	3366	NH2 ARG	697	38.014	34.643	76.318	1.00	18.93 7
ATOM	3367	C ARG	697	41.625	40.494	73.818	1.00	18.98 6
ATOM	3368	O ARG	697	41.180	40.255	72.677	1.00	19.20 8
ATOM	3369	N ALA	698	42.926	40.660	74.077	1.00	17.10 7
ATOM	3370	CA ALA	698	43.973	40.609	73.057	1.00	14.99 5
ATOM	3371	CB ALA	698	44.816	41.858	73.146	1.00	15.98 6
ATOM	3372	C ALA	698	44.838	39.366	73.296	1.00	14.49 6
ATOM	3373	O ALA	698	45.073	38.999	74.432	1.00	16.90 8
ATOM	3374	N ARG	699	45.349	38.753	72.234	1.00	13.57 7
ATOM	3375	CA ARG	699	46.174	37.540	72.325	1.00	10.72 5
ATOM	3376	CB ARG	699	45.229	36.331	72.392	1.00	12.04 6
ATOM	3377	CG ARG	699	45.692	35.014	71.794	1.00	12.63 6
ATOM	3378	CD ARG	699	46.738	34.349	72.665	1.00	20.39 6
ATOM	3379	NE ARG	699	46.913	32.910	72.399	1.00	21.37 7
ATOM	3380	CZ ARG	699	46.119	31.955	72.895	1.00	21.92 6
ATOM	3381	NH1 ARG	699	45.069	32.257	73.672	1.00	21.47 7
ATOM	3382	NH2 ARG	699	46.442	30.682	72.710	1.00	22.33 7
ATOM	3383	C ARG	699	47.090	37.470	71.094	1.00	9.38 6
ATOM	3384	O ARG	699	46.680	37.820	69.991	1.00	10.86 8
ATOM	3385	N MET	700	48.355	37.109	71.282	1.00	8.21 7
ATOM	3386	CA MET	700	49.263	37.029	70.140	1.00	7.21 6
ATOM	3387	CB MET	700	50.724	36.955	70.551	1.00	6.01 6
ATOM	3388	CG MET	700	51.322	38.292	70.963	1.00	5.33 5
ATOM	3389	SD MET	700	52.092	39.250	69.678	1.00	9.84 16
ATOM	3390	CE MET	700	51.368	40.792	69.955	1.00	8.49 5
ATOM	3391	C MET	700	48.875	35.808	69.375	1.00	6.64 6
ATOM	3392	O MET	700	48.609	34.755	69.939	1.00	6.32 8
ATOM	3393	N ALA	701	48.849	35.943	68.069	1.00	7.50 7
ATOM	3394	CA ALA	701	48.425	34.837	67.250	1.00	8.94 6
ATOM	3395	CB ALA	701	47.605	35.361	66.065	1.00	7.41 6
ATOM	3396	C ALA	701	49.483	33.855	66.779	1.00	9.12 6
ATOM	3397	O ALA	701	50.679	34.165	66.639	1.00	9.86 3
ATOM	3398	N GLU	702	48.980	32.669	66.491	1.00	10.01 7
ATOM	3399	CA GLU	702	49.763	31.574	65.587	1.00	15.16 6
ATOM	3400	CB GLU	702	48.971	30.275	66.108	1.00	15.92 6
ATOM	3401	CG GLU	702	48.724	29.784	67.501	1.00	18.17 6
ATOM	3402	CD GLU	702	48.597	28.284	67.507	1.00	21.01 5
ATOM	3403	OE1 GLU	702	47.904	27.731	66.611	1.00	22.10 8
ATOM	3404	OE2 GLU	702	49.233	27.652	68.377	1.00	24.81 8
ATOM	3405	C GLU	702	50.126	31.770	64.510	1.00	13.07 6
ATOM	3406	O GLU	702	49.560	32.617	63.802	1.00	12.10 8
ATOM	3407	N PRO	703	51.106	30.986	64.037	1.00	14.95 7
ATOM	3408	CD PRO	703	51.501	30.820	62.625	1.00	17.31 6
ATOM	3409	CA PRO	703	51.782	30.007	64.899	1.00	14.84 5
ATOM	3410	CB PRO	703	51.896	28.794	63.999	1.00	14.77 6
ATOM	3411	CG PRO	703	52.253	29.467	62.635	1.00	19.35 6
ATOM	3412	C PRO	703	53.150	30.488	65.409	1.00	13.50 5
ATOM	3413	O PRO	703	53.801	29.774	66.157	1.00	15.09 8
ATOM	3414	N SER	704	53.587	31.681	65.002	1.00	11.82 7
ATOM	3415	CA SER	704	54.873	32.218	65.461	1.00	9.78 5
ATOM	3416	CB SER	704	55.156	33.574	64.798	1.00	9.23 5
ATOM	3417	CG SER	704	55.301	33.474	63.394	1.00	8.65 8
ATOM	3418	C SER	704	54.860	32.386	67.003	1.00	11.09 6
ATOM	3419	O SER	704	55.621	31.729	67.736	1.00	12.01 8
ATOM	3420	N PHE	705	53.937	33.229	67.468	1.00	8.75 7
ATOM	3421	CA PHE	705	53.767	33.532	68.857	1.00	3.52 6
ATOM	3422	CB PHE	705	53.323	34.973	68.988	1.00	5.09 6
ATOM	3423	CG PHE	705	54.159	35.924	68.184	1.00	7.49 5
ATOM	3424	CD1 PHE	705	53.696	36.417	66.957	1.00	8.92 5



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ATOM	3425	CD2	PHE	705	55.446	36.284	68.611	1.00	8.54	1
ATOM	3426	CE1	PHE	705	54.512	37.252	66.163	1.00	7.44	2
ATOM	3427	CE2	PHE	705	56.270	37.115	67.833	1.00	4.91	3
ATOM	3428	CZ	PHE	705	55.804	37.598	66.606	1.00	5.19	4
ATOM	3429	C	PHE	705	52.783	32.591	69.505	1.00	5.11	5
ATOM	3430	O	PHE	705	52.257	31.697	68.878	1.00	4.57	6
ATOM	3431	N	GLY	706	52.634	32.751	70.809	1.00	8.69	7
ATOM	3432	CA	GLY	706	51.728	31.956	71.622	1.00	7.99	8
ATOM	3433	C	GLY	706	51.661	32.726	72.932	1.00	9.39	9
ATOM	3434	O	GLY	706	52.345	33.739	73.069	1.00	9.05	10
ATOM	3435	N	GLY	707	50.829	32.295	73.878	1.00	10.91	11
ATOM	3436	CA	GLY	707	50.738	32.990	75.162	1.00	9.27	12
ATOM	3437	C	GLY	707	49.465	32.823	75.977	1.00	7.80	13
ATOM	3438	O	GLY	707	48.894	31.731	76.063	1.00	7.37	14
ATOM	3439	N	PHE	708	48.993	33.927	76.540	1.00	7.59	15
ATOM	3440	CA	PHE	708	47.801	33.911	77.372	1.00	8.42	16
ATOM	3441	CB	PHE	708	48.171	33.981	78.874	1.00	9.14	17
ATOM	3442	CG	PHE	708	49.358	33.126	79.277	1.00	8.19	18
ATOM	3443	CD1	PHE	708	49.196	31.787	79.592	1.00	5.98	19
ATOM	3444	CD2	PHE	708	50.638	33.679	79.352	1.00	6.32	20
ATOM	3445	CE1	PHE	708	50.296	31.016	79.974	1.00	8.74	21
ATOM	3446	CE2	PHE	708	51.730	32.912	79.731	1.00	5.05	22
ATOM	3447	CZ	PHE	708	51.570	31.587	80.040	1.00	4.00	23
ATOM	3448	C	PHE	708	46.846	35.066	77.077	1.00	7.99	24
ATOM	3449	O	PHE	708	47.260	36.187	76.721	1.00	6.94	25
ATOM	3450	N	TRP	709	45.562	34.777	77.285	1.00	9.09	26
ATOM	3451	CA	TRP	709	44.475	35.752	77.119	1.00	12.14	27
ATOM	3452	CB	TRP	709	43.114	35.083	77.396	1.00	11.59	28
ATOM	3453	CG	TRP	709	42.417	34.592	76.165	1.00	12.07	29
ATOM	3454	CD2	TRP	709	42.098	35.354	74.999	1.00	9.80	30
ATOM	3455	CE2	TRP	709	41.465	34.481	74.092	1.00	9.82	31
ATOM	3456	CE3	TRP	709	42.283	36.687	74.634	1.00	9.79	32
ATOM	3457	CD1	TRP	709	41.971	33.326	75.929	1.00	11.53	33
ATOM	3458	NE1	TRP	709	41.398	33.250	74.688	1.00	12.13	34
ATOM	3459	CZ2	TRP	709	41.018	34.897	72.841	1.00	9.03	35
ATOM	3460	CZ3	TRP	709	41.838	37.103	73.399	1.00	11.59	36
ATOM	3461	CH2	TRP	709	41.214	36.209	72.513	1.00	10.54	37
ATOM	3462	C	TRP	709	44.635	36.973	78.056	1.00	10.56	38
ATOM	3463	O	TRP	709	44.770	36.823	79.268	1.00	12.13	39
ATOM	3464	N	SER	710	44.620	38.177	77.508	1.00	11.52	40
ATOM	3465	CA	SER	710	44.765	39.350	78.351	1.00	12.14	41
ATOM	3466	CB	SER	710	45.040	40.594	77.501	1.00	9.78	42
ATOM	3467	OG	SER	710	43.847	41.258	77.157	1.00	10.05	43
ATOM	3468	C	SER	710	43.522	39.567	79.216	1.00	12.22	44
ATOM	3469	O	SER	710	42.531	38.832	79.139	1.00	17.16	45
ATOM	3470	N	ALA	711	43.580	40.563	80.076	1.00	12.01	46
ATOM	3471	CA	ALA	711	42.435	40.867	80.894	1.00	12.49	47
ATOM	3472	CB	ALA	711	42.855	41.817	81.993	1.00	12.98	48
ATOM	3473	C	ALA	711	41.432	41.560	79.965	1.00	13.23	49
ATOM	3474	O	ALA	711	41.810	42.073	78.915	1.00	14.99	50
ATOM	3475	N	TRP	712	40.155	41.558	80.326	1.00	13.85	51
ATOM	3476	CA	TRP	712	39.159	42.251	79.527	1.00	12.59	52
ATOM	3477	CB	TRP	712	37.751	42.031	80.092	1.00	8.73	53
ATOM	3478	CG	TRP	712	37.202	40.647	79.845	1.00	8.57	54
ATOM	3479	CD2	TRP	712	36.796	40.091	78.576	1.00	8.04	55
ATOM	3480	CE2	TRP	712	36.416	38.745	78.809	1.00	8.30	56
ATOM	3481	CE3	TRP	712	36.718	40.600	77.270	1.00	4.78	57
ATOM	3482	CD1	TRP	712	37.037	39.647	80.769	1.00	8.29	58
ATOM	3483	NE1	TRP	712	36.574	38.499	80.150	1.00	8.70	59
ATOM	3484	CZ2	TRP	712	35.969	37.906	77.783	1.00	8.46	60
ATOM	3485	CZ3	TRP	712	36.279	39.776	76.262	1.00	7.52	61
ATOM	3486	CH2	TRP	712	35.908	38.434	76.520	1.00	9.00	62
ATOM	3487	C	TRP	712	39.498	43.747	79.520	1.00	12.59	63
ATOM	3488	O	TRP	712	40.124	44.269	80.460	1.00	12.30	64
ATOM	3489	N	SER	713	39.174	44.385	78.395	1.00	15.22	65
ATOM	3490	CA	SER	713	39.366	45.819	78.166	1.00	15.45	66
ATOM	3491	CB	SER	713	39.294	46.108	76.659	1.00	14.50	67
ATOM	3492	OG	SER	713	37.973	45.899	76.149	1.00	11.86	68
ATOM	3493	C	SER	713	38.167	46.480	78.799	1.00	15.86	69
ATOM	3494	O	SER	713	37.081	45.908	78.764	1.00	18.64	70
ATOM	3495	N	GLU	714	38.309	47.705	79.279	1.00	17.04	71
ATOM	3496	CA	GLU	714	37.163	48.391	79.888	1.00	20.29	72
ATOM	3497	CB	GLU	714	37.524	49.809	80.276	1.00	21.54	73
ATOM	3498	CG	GLU	714	38.470	49.836	81.447	1.00	24.61	74
ATOM	3499	CD	GLU	714	38.699	51.236	81.978	1.00	26.47	75
ATOM	3500	OE1	GLU	714	39.860	51.479	82.420	1.00	27.51	76
ATOM	3501	OE2	GLU	714	37.735	52.074	81.957	1.00	25.69	77
ATOM	3502	C	GLU	714	35.885	48.366	79.027	1.00	21.46	78

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ATOM	3503	O	GLU	714	33.867	48.844	77.886	1.00	21.24	3	
ATOM	3504	N	PRO	715	34.787	47.832	79.611	1.00	20.46	7	
ATOM	3505	CD	PRO	715	34.703	47.767	81.090	1.00	21.13	5	
ATOM	3506	CA	PRO	715	33.460	47.694	79.015	1.00	19.23	5	
ATOM	3507	CB	PRO	715	32.627	47.183	80.182	1.00	21.32	5	
ATOM	3508	CG	PRO	715	33.226	47.974	81.352	1.00	19.98	5	
ATOM	3509	C	PRO	715	32.874	48.959	78.473	1.00	20.02	5	
ATOM	3510	O	PRO	715	33.194	50.060	78.922	1.00	20.10	3	
ATOM	3511	N	VAL	716	31.934	48.769	77.562	1.00	20.51	7	
ATOM	3512	CA	VAL	716	31.229	49.858	76.910	1.00	19.79	5	
ATOM	3513	CB	VAL	716	31.769	50.100	75.440	1.00	18.56	5	
ATOM	3514	CG1	VAL	716	30.988	49.293	74.396	1.00	18.80	5	
ATOM	3515	CG2	VAL	716	31.749	51.563	75.099	1.00	16.95	5	
ATOM	3516	C	VAL	716	29.778	49.366	76.908	1.00	21.79	5	
ATOM	3517	O	VAL	716	29.515	48.182	76.624	1.00	20.72	3	
ATOM	3518	N	SER	717	28.859	50.269	77.264	1.00	22.27	7	
ATOM	3519	CA	SER	717	27.439	49.971	77.331	1.00	21.09	5	
ATOM	3520	CB	SER	717	26.920	50.181	78.764	1.00	23.89	6	
ATOM	3521	OG	SER	717	27.182	49.064	79.607	1.00	24.17	8	
ATOM	3522	C	SER	717	26.552	50.748	76.375	1.00	20.65	6	
ATOM	3523	O	SER	717	26.541	51.970	76.394	1.00	19.78	3	
ATOM	3524	N	LEU	718	25.838	50.014	75.523	1.00	21.29	7	
ATOM	3525	CA	LEU	718	24.866	50.583	74.585	1.00	21.71	6	
ATOM	3526	CB	LEU	718	25.009	49.949	73.188	1.00	17.72	5	
ATOM	3527	CG	LEU	718	24.502	50.860	72.057	1.00	15.29	5	
ATOM	3528	CD1	LEU	718	25.271	52.197	72.069	1.00	11.08	6	
ATOM	3529	CD2	LEU	718	24.631	50.165	70.733	1.00	11.73	5	
ATOM	3530	C	LEU	718	23.477	50.236	75.183	1.00	22.58	5	
ATOM	3531	O	LEU	718	23.399	49.506	76.191	1.00	24.55	3	
ATOM	3532	N	LEU	719	22.392	50.723	74.564	1.00	23.55	7	
ATOM	3533	CA	LEU	719	21.023	50.470	75.054	1.00	23.37	5	
ATOM	3534	CB	LEU	719	20.632	51.986	76.069	1.00	23.00	6	
ATOM	3535	CG	LEU	719	21.540	51.746	77.325	1.00	22.19	6	
ATOM	3536	CD1	LEU	719	21.290	53.039	78.084	1.00	19.79	5	
ATOM	3537	CD2	LEU	719	21.416	50.545	78.254	1.00	20.88	6	
ATOM	3538	C	LEU	719	19.986	50.393	73.904	1.00	23.18	6	
ATOM	3539	O	LEU	719	18.886	50.958	74.036	1.00	24.17	8	
ATOM	3540	N	THR	720	20.325	49.657	72.828	1.00	22.42	7	
ATOM	3541	CA	THR	720	19.498	49.515	71.597	1.00	21.89	6	
ATOM	3542	CB	THR	720	19.038	48.042	71.295	1.00	22.47	6	
ATOM	3543	OG1	THR	720	18.798	47.332	72.513	1.00	24.25	8	
ATOM	3544	CG2	THR	720	20.042	47.288	70.444	1.00	20.74	5	
ATOM	3545	C	THR	720	18.263	50.417	71.492	1.00	22.94	5	
ATOM	3546	O	THR	720	17.140	49.947	71.240	1.00	22.69	3	



Table 2

Peptide1-EBP1	Peptide1-EBP2	Peptide1-EBP2	Peptide2-EBP1	Peptide1-Peptide2
Gly <sup>P9</sup> O-Met <sup>150</sup> N	Tyr <sup>P4</sup> OH-Ser <sup>92</sup> N	Gly <sup>P9</sup> O-Met <sup>150</sup> N	Tyr <sup>P4</sup> OH-Ser <sup>92</sup> N	Tyr <sup>P4</sup> O-Cys <sup>P6</sup> N
Pro <sup>P10</sup> O-Thr <sup>151</sup> N		Pro <sup>P10</sup> O-Thr <sup>151</sup> N		Tyr <sup>P4</sup> N-Cys <sup>P6</sup> O
Pro <sup>P10</sup> O-Thr <sup>151</sup> Oγ		Pro <sup>P10</sup> O-Thr <sup>151</sup> Oγ1		Cys <sup>P6</sup> O-Tyr <sup>P4</sup> N
Leu <sup>P11</sup> O-Ser <sup>152</sup> N		Leu <sup>P11</sup> O-Ser <sup>152</sup> N		Cys <sup>P6</sup> N-Tyr <sup>P4</sup> O
Leu <sup>P11</sup> O-Ser <sup>152</sup> Oγ		Leu <sup>P11</sup> O-Ser <sup>152</sup> Oγ		

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**CLAIMS**

What is claimed is:

1. A computer-assisted method for identifying potential mimetics of erythropoietin, using a programmed computer comprising a processor, a data storage system, an input device, and an output device, comprising the steps of:
  - 5 (a) inputting into the programmed computer through said input device data comprising the three-dimensional coordinates of a subset of the atoms in the peptide GGTYSCHFGLTWVCKPQGG when said peptide is co-crystallized with a portion of the erythropoietin receptor comprising amino acids 1 to 225 of said receptor, thereby generating a criteria data set;
  - 10 (b) comparing, using said processor, said criteria data set to a computer database of chemical structures stored in said computer data storage system;
  - (c) selecting from said database, using computer methods, chemical structures having a portion that is structurally similar to said criteria data set;
  - 15 (d) outputting to said output device the selected chemical structures having a portion similar to said criteria data set.

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2. A computer-assisted method for identifying potential mimetics of erythropoietin, using a programmed computer comprising a processor, a data storage system, an input device, and an output device, comprising the steps of:
  - 5 (a) inputting into the programmed computer through said input device data comprising the three-dimensional coordinates of a subset of the atoms in the peptide GGTYSCHFGPLTWVCKPQGG when said peptide is co-crystallized with a portion of the erythropoietin receptor comprising amino acids 1 to 225 of said receptor, thereby generating a criteria data set;
  - 10 (b) constructing, using computer methods, a model of a chemical structure having a portion that is structurally similar to said criteria data set;
  - (c) outputting to said output device the constructed model.
3. A compound having a chemical structure selected using the method of claim 1,  
15 said compound being an EPO mimetic.
4. The compound of claim 3 wherein said compound is not a peptide.
5. The compound of claim 3 wherein said compound is a peptide.  
20
6. The compound of claims 5 wherein said peptide has 15 or fewer amino acids.

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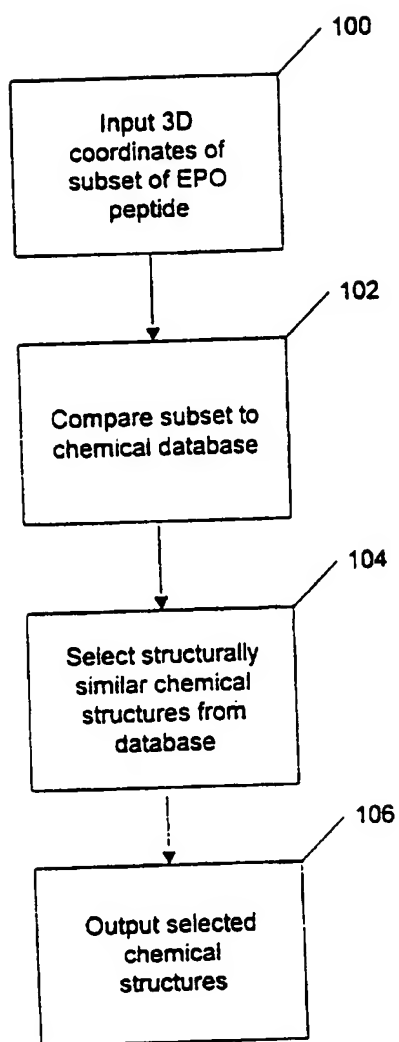


FIG. 1

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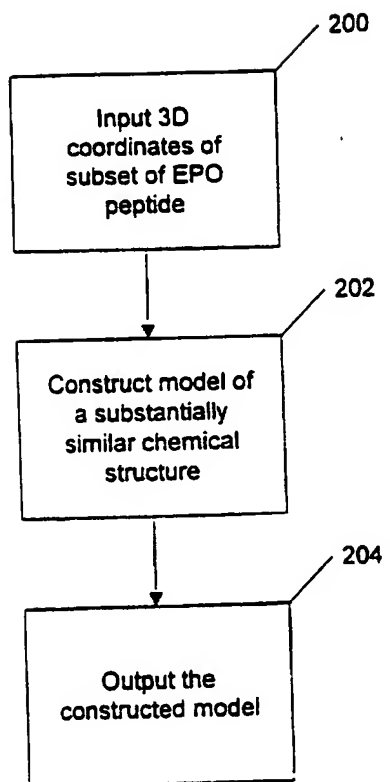


FIG. 2



## INTERNATIONAL SEARCH REPORT

International application No.  
PCT/US97/07218

## A. CLASSIFICATION OF SUBJECT MATTER

IPC(6) :G06F 159:00

US CL :364/496

According to International Patent Classification (IPC) or to both national classification and IPC

## B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)

U.S. : 364/496, 497,498,578

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

Electronic data base consulted during the international search (name of data base and, where practicable, search terms used)

aps, dialog

search terms: erythropoietin, receptor, 3d, pdb or database

## C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category*	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
X	US, 5,331,573 A (BALAJI et al.) 19 July 1994, (col. 7, lines 46-66, col. 13, lines 20-55, col. 14, lines 12-23	1-6
A,P	US 5,557,535 A (SRINIVASAN et al.) 17 September 1996, (abstract, fig. 1, col. 4, line 57 - col. 6, line 55)	1,2
A,P	US 5,555,366 A (TEIG et al.) 10 September 1996, (abstract, fig. 8, fig. 12)	1,2
A	US 5,265,030 A (SKOLNICK et al.) 23 November 1993, (col. 2, line 20 - col. 3, line 20)	1,2
A,P	MCCARTHY, "Small Peptide Designed that can Mimic Erythropoietin" Lancet, 8/96 vol. 348, no. 24, p.395	1-6



Further documents are listed in the continuation of Box C.



See patent family annex.

* Special categories of cited documents:	*T	later document published after the international filing date or priority date and not in conflict with the application but cited to understand the principle or theory underlying the invention
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*E* earlier document published on or after the international filing date	*Y*	document of particular relevance; the claimed invention cannot be considered to involve an inventive step when the document is combined with one or more other such documents, such combination being obvious to a person skilled in the art
*L* document which may throw doubts on priority claim(s) or which is cited to establish the publication date of another citation or other special reason (as specified)	*A*	document member of the same patent family
*O* document referring to an oral disclosure, use, exhibition or other means		
*P* document published prior to the international filing date but later than the priority date claimed		

Date of the actual completion of the international search

05 JULY 1997

Date of mailing of the international search report

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**INTERNATIONAL SEARCH REPORT**International application No.  
PCT/US97/07218**C (Continuation). DOCUMENTS CONSIDERED TO BE RELEVANT**

Category*	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
X,P	LIVNAH ET AL., "Functional Mimicry of a Protein Hormone by a Peptide Agonist" Science 26 July 1996, vol. 273 no. 274, p. 464-471.	1-6